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NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	JAN 27	Source of Registration (SR) information in REGISTRY updated and searchable
NEWS	4	JAN 27	A new search aid, the Company Name Thesaurus, available in CA/CAplus
NEWS	5	FEB 05	German (DE) application and patent publication number format changes
NEWS	6	MAR 03	MEDLINE and LMEDLINE reloaded
NEWS	7	MAR 03	MEDLINE file segment of TOXCENTER reloaded
NEWS	8	MAR 03	FRANCEPAT now available on STN
NEWS	9	MAR 29	Pharmaceutical Substances (PS) now available on STN
NEWS	10	MAR 29	WPIFV now available on STN
NEWS	11	MAR 29	No connect hour charges in WPIFV until May 1, 2004
NEWS	12	MAR 29	New monthly current-awareness alert (SDI) frequency in RAPRA

NEWS EXPRESS	MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 13 APRIL 2004
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
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FILE 'HOME' ENTERED AT 17:04:15 ON 22 APR 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 17:04:28 ON 22 APR 2004
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STRUCTURE FILE UPDATES: 21 APR 2004 HIGHEST RN 676437-01-7
DICTIONARY FILE UPDATES: 21 APR 2004 HIGHEST RN 676437-01-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
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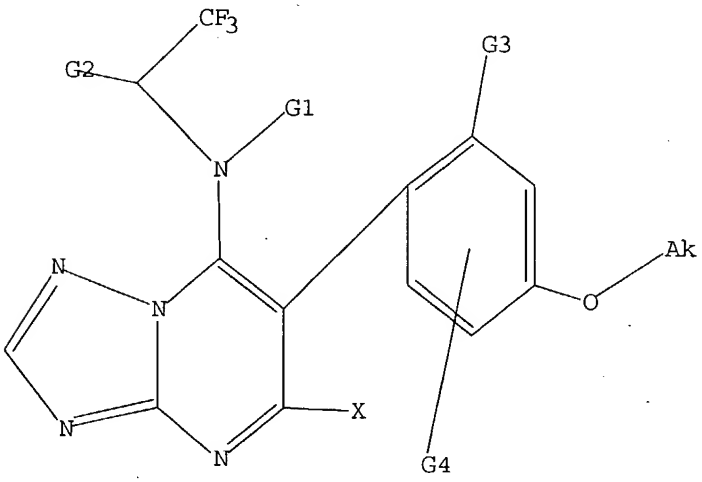
L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 H,Ak

G2 H,Me

G3 MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,s-BuO,t-BuO,PhO,NO2

G4 X,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full

FULL SEARCH INITIATED 17:05:03 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 4 TO ITERATE

100.0% PROCESSED 4 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L2 0 SEA SSS FUL L1

=> file marpat

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	155.42	155.63

FILE 'MARPAT' ENTERED AT 17:05:12 ON 22 APR 2004
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FILE CONTENT: 1988-PRESENT (VOL 140 ISS 16)(20040416/ED)

MOST RECENT CITATIONS FOR PATENTS FROM FIVE MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US 6706759 16 MAR 2004
DE 10335606 11 MAR 2004
EP 1396268 10 MAR 2004
JP 2004095205 25 MAR 2004
WO 2004022766 18 MAR 2004

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

=> s l1 sss full
FULL SEARCH INITIATED 17:05:19 FILE 'MARPAT'
FULL SCREEN SEARCH COMPLETED - 68 TO ITERATE

100.0% PROCESSED 68 ITERATIONS 6 ANSWERS
SEARCH TIME: 00.00.06

L3 6 SEA SSS FUL L1

=> file caold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	109.42	265.05

FILE 'CAOLD' ENTERED AT 17:05:32 ON 22 APR 2004
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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts

printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> s l1 sss full
REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 17:05:38 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 4 TO ITERATE

100.0% PROCESSED 4 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L4 0 SEA SSS FUL L1

L5 0 L4

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.42	421.31

FILE 'CAPLUS' ENTERED AT 17:05:46 ON 22 APR 2004
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FILE COVERS 1907 - 22 Apr 2004 VOL 140 ISS 17
FILE LAST UPDATED: 21 Apr 2004 (20040421/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L6 0 L2

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=> s l3
L7            6 L3

=> d his

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     FILE 'REGISTRY' ENTERED AT 17:04:28 ON 22 APR 2004
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L2            0 S L1 SSS FULL

     FILE 'MARPAT' ENTERED AT 17:05:12 ON 22 APR 2004
L3            6 S L1 SSS FULL

     FILE 'CAOLD' ENTERED AT 17:05:32 ON 22 APR 2004
                S L1

     FILE 'REGISTRY' ENTERED AT 17:05:37 ON 22 APR 2004
L4            0 S L1 SSS FULL

     FILE 'CAOLD' ENTERED AT 17:05:39 ON 22 APR 2004
L5            0 S L4 SSS FULL

     FILE 'CAPLUS' ENTERED AT 17:05:46 ON 22 APR 2004
L6            0 S L2
L7            6 S L3

=> d l7 fbib hitstr abs total

L7   ANSWER 1 OF 6  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   2003:76783  CAPLUS
DN   138:137323
TI   Substituted 6-(2-tolyl)-triazolo[1,5-a]pyrimidines as fungicides
IN   Tormo i Blasco, Jordi; Sauter, Hubert; Mueller, Bernd; Gewehr, Markus;
     Grammenos, Wassilios; Grote, Thomas; Gypser, Andreas; Rheinheimer,
     Joachim; Rose, Ingo; Schaefer, Peter; Schieweck, Frank; Rack, Michael;
     Ammermann, Eberhard; Strathmann, Siegfried; Lorenz, Gisela; Stierl,
     Reinhard
PA   BASF Aktiengesellschaft, Germany; et al.
SO   PCT Int. Appl., 49 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.        KIND  DATE          APPLICATION NO.  DATE
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PI   WO 2003008417      A1   20030130      WO 2002-EP7578   20020708
     WO 2003008417      C2   20031030
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
             TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
             CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
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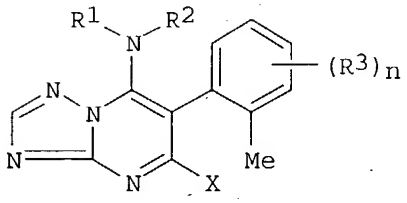
PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 2001-117402 A 20010718

OS MARPAT 138:137323

GI



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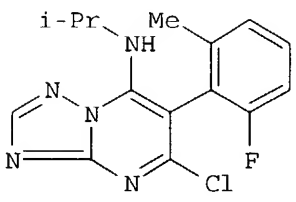

II

AB Title compds. I [R1-2 = H, alk(en/yn)yl, alkadienyl, etc.; R3 = halo, CN, alkyl, alkoxy, haloalkyl, etc.; n = 1-4; X = halo, CN, alkyl, alkoxy, etc.] are prepared For instance, 3-amino-1,2,4-triazole and di-Et (2-fluoro-6-methylphenyl)malonate (preparation given) are reacted (n-Bu3N, 180°, 6 h) and the intermediate treated with NaOH to give 5,7-dihydroxy-6-(2-fluoro-6-methylphenyl)-[1,2,4]triazolo[1,5-a]pyrimidine. This is converted to the dichloro derivative (POCl3, reflux, 8 h) and reacted with i-PrNH2 (Et3N, CH2Cl2) to yield II. Several example compds. at 63 ppm gave 97% control of Altenaria solani on tomato. I are useful for combating phytopathogenic fungi.

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:31452 CAPLUS

DN **136:96032**

TI Substituted triazolopyrimidines as anticancer agents

IN Schmitt, Mark R.; Kirsch, Donald R.; Harris, Jane E.; Beyer, Carl F.; Pees, Klaus-Juergen; Carter, Paul; Pfrengle, Waldemar; Albert, Guido

PA American Home Products Corporation, USA

SO PCT Int. Appl., 405 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002002563	A2	20020110	WO 2001-US20672	20010628
WO 2002002563	A3	20030103		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 2000-215585PP 20000630

BR 2001012038	A	20030401	BR 2001-12038	20010628
			US 2000-215585PP	20000630
			WO 2001-US20672W	20010628
EP 1307200	A2	20030507	EP 2001-952295	20010628
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
			US 2000-215585PP	20000630
			WO 2001-US20672W	20010628
JP 2004502691	T2	20040129	JP 2002-507815	20010628
			US 2000-215585PP	20000630
			WO 2001-US20672W	20010628
US 2002068744	A1	20020606	US 2001-895975	20010629
			US 2000-215585PP	20000630
NO 2002006195	A	20030227	NO 2002-6195	20021223
			US 2000-215585PP	20000630
			WO 2001-US20672W	20010628

OS MARPAT 136:96032

AB A method is provided for treating or inhibiting the growth of cancerous tumor cells and associated diseases in a mammal in need thereof which comprises administering to the mammal an effective amount of a substituted triazolopyrimidine derivative or a pharmaceutically acceptable salt thereof. Also provided is a method for treating or inhibiting the growth of cancerous tumor cells and associated diseases in a mammal in need thereof by interacting with tubulin and microtubules and promoting microtubule polymerization which comprises administering to the mammal an effective amount of a substituted triazolopyrimidine derivative or a pharmaceutically acceptable salt thereof.

L7 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:195201 CAPLUS
DN **134:233069**
TI Preparation of optically active fungicidal trifluoromethylalkylamino-triazolopyrimidines
IN Pfrengle, Waldemar; Pees, Klaus-Juergen; Albert, Guido; Carter, Paul; Rehnig, Annerose; Cotter, Henry Van Tuyl
PA American Cyanamid Co., USA
SO U.S., 11 pp., Cont.-in-part of U.S. 5,986,135.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6204269	B1	20010320	US 1999-406574	19990924
				US 1998-160894 A2	19980925
	US 5986135	A	19991116	US 1998-160894	19980925

PATENT FAMILY INFORMATION:
FAN 1999:733059

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5986135	A	19991116	US 1998-160894	19980925
	ZA 9905673	A	20000330	ZA 1999-5673	19990902
				US 1998-160894 A	19980925
	JP 2000119275	A2	20000425	JP 1999-265647	19990920
				US 1998-160894 A	19980925
	KR 2000023437	A	20000425	KR 1999-41162	19990922
				US 1998-160894 A	19980925

EP 989130		A1	20000329	EP 1999-307522	19990923
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
				US 1998-160894 A	19980925
BR 9904354		A	20000912	BR 1999-4354	19990923
				US 1998-160894 A	19980925
CN 1250052		A	20000412	CN 1999-120740	19990924
				US 1998-160894 A	19980925
US 6204269		B1	20010320	US 1999-406574	19990924
				US 1998-160894 A2	19980925

OS MARPAT 134:233069
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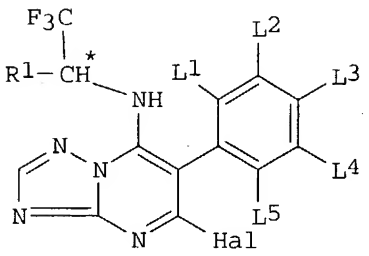


I

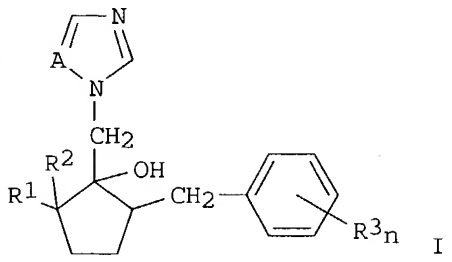
AB Optically active 7-(1,1,1-trifluoroalk-2-ylamino)-triazolopyrimidines I (R1 = C2-C6 alkyl; CH* = chiral carbon atom; Hal = halo; L1-L5 = H, halo, alkyl, alkoxy, or nitro), characterized in that the enantiomeric excess of the (S)-enantiomer is at least 70%, are prepared and show enhanced selective fungicidal activity against phytopathogenic fungi. The new compds. are processed with carriers, and optionally with adjuvants, to form fungicidal compns.

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:534806 CAPLUS
DN **133:131170**
TI Nonaqueous emulsifiable concentrate fungicide formulation
IN Aven, Michael
PA American Cyanamid Co., USA
SO Eur. Pat. Appl., 15 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI EP 1023837	A2	20000802	EP 2000-300666	20000128
EP 1023837	A3	20010530		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
			US 1999-240634 A	19990129

OS MARPAT 133:131170
GI



I

AB The title formulation comprises 50-300 g/L azole derivative I [R1, R2 = H or (un)substituted alkyl, alkenyl, alkynyl or alkadienyl; R3 = halo or (un)substituted alkyl, alkenyl, alkynyl, alkadienyl, alkoxy or aryl; A = N or CH; n = 0,1 or 2] and, optionally, 50-500 g/L addnl. fungicide, as active ingredient. The inactive formulation ingredients are ≥700 g/L alkoxylates of an aliphatic alc., ≤100 g/L nonionic dispersant(s), 10-100 g/L anionic dispersant(s), 50-600 g/L polar aprotic organic solvent(s), 150-500 g/L nonpolar organic solvent(s), and ≤5 g/L defoamer.

L7 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:534803 CAPLUS
DN **133:131168**
TI Synergistic fungicidal mixtures
IN Van Tuyl Cotter, Henry; Reichert, Gunter; Sieverding, Ewald; Jegerings, Petrus Martinus Franciscus Emanuel
PA American Cyanamid Co., USA; BASF AG
SO Eur. Pat. Appl., 48 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1023834	A1	20000802	EP 2000-300637	20000128
	EP 1023834	B1	20040407		
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				US 1999-117725PP	19990129
				US 1999-240412 A	19990129
	US 6346535	B1	20020212	US 1999-240412	19990129
	US 6521628	B1	20030218	US 2000-492440	20000127
				US 1999-117725PP	19990129
	US 2002099062	A1	20020725	US 2002-46190	20020116
	US 6498194	B2	20021224		
				US 1999-240412 A1	19990129
	US 2002099063	A1	20020725	US 2002-46197	20020116
				US 1999-240412 A1	19990129

OS MARPAT 133:131168
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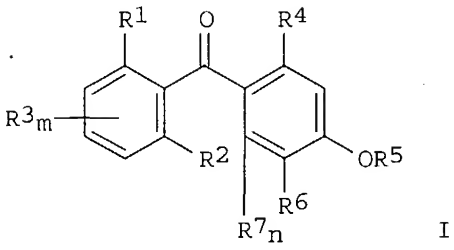

I

AB The title compns. comprise a benzophenone derivative mixted with at least one fungicide selected from a ergosterol biosynthesis inhibitor, a strobilurine derivative, a melanin biosynthesis inhibitor, a compound selected from acibenzolar, benomyl, captan, carboxin, chlorothalonil, copper, cyprodinil, dinocap, dithianon, dimethomorph, dodine, ethirimol, famoxadone, fenpiclonil, fluazinam, mancozeb, metalaxyl, pyrifenox, sulfur, vinclozolin, and/or an azolopyrimidine derivative (Markush given). The benzophenone derivative is I [R1 = OH, halo or (un)substituted alkyl, alkanoyloxy or alkoxy; R2 = halo or (un)substituted alkyl; R3 = halo, NO2 or (un)substituted alkyl or alkoxy; R4 = halo, CN, OH, CO2H, NH2, NO2, or (un)substituted alkyl, alkoxy, alkenyl, alkylthio, alkylsulfinyl or alkylsulfonyl; R5 = (un)substituted alkyl;R6 = halo, NO2, (un)substituted alkyl, alkoxy, aryloxy, etc.; R7 = halo, (un)substituted (cyclo)alkyl, alkenyl, (cyclo)alkoxy, etc.; m - o, 1-3; n = 0 or 1].
RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:708827 CAPLUS
DN **129:302657**
TI Preparation of fungicidal [trifluoromethyl(alkyl)amino]triazolopyrimidines
IN Pees, Klaus-Juergen; Krummel, Guenter; Van Tuyl Cotter, Henry; Rehnig, Annerose; May, Leslie; Pfrengle, Waldemar; Albert, Guido
PA American Cyanamid Co., USA
SO PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9846608	A1	19981022	WO 1998-US5615	19980323
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	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
				US 1997-843323 A	19970414
				US 1998-150572 A	19980910
	TW 460476	B	20011021	TW 1998-87103847	19980316
				US 1997-843323 A	19970414
	AU 9868671	A1	19981111	AU 1998-68671	19980323
	AU 735730	B2	20010712		

			US 1997-843323 A 19970414
			WO 1998-US5615 W 19980323
EP 975635	A1	20000202	EP 1998-914274 19980323
EP 975635	B1	20030507	
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			US 1997-843323 A 19970414
			WO 1998-US5615 W 19980323
BR 9808531	A	20000523	BR 1998-8531 19980323
			US 1997-843323 A 19970414
			WO 1998-US5615 W 19980323
EE 9900486	A	20000615	EE 1999-486 19980323
			US 1997-843323 A 19970414
			WO 1998-US5615 W 19980323
NZ 500143	A	20010629	NZ 1998-500143 19980323
			US 1997-843323 A 19970414
			WO 1998-US5615 W 19980323
JP 2001520650	T2	20011030	JP 1998-543913 19980323
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OS MARPAT 129:302657
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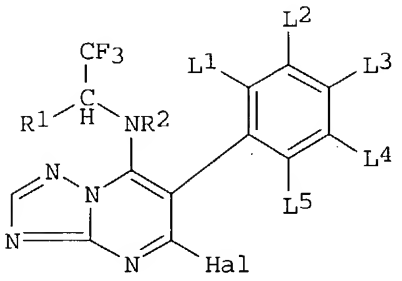

I

AB The title compds. [I; R1, R2 = H, (un)substituted alk(en)yl, alkynyl, alkadienyl or Ph; Hal = halo; L1-L5 = H, halo, alkyl, alkoxy, NO2], fungicides with selective activity, were prepared by amination of 5,7-dihalo-6-phenyltriazolopyrimidines with trifluoroalkylamines. The new compds. are processed with carriers and adjuvants to fungicidal compns. For example, a stirred mixture of 1.4 mmol 5,7-dichloro-6-(2-chloro-6-fluorophenyl)-1,2,4-triazolo[1.5a]pyrimidine with 30 mL CH2Cl2 was treated with a mixture of 4.2 mmol CF3CH2NH2 and 10 mL CH2Cl2 and the whole was stirred for 16 h at ambient temperature to give I (R2 = L2 = L3 = L4 = H, L5 = F) (II; R1 = H, L1 = Cl). II (R1 = Me, L1 = F) (III) inhibited mycelial growth of Alternaria solani and Rhizoctonia solani with MIC 0.78 and 3.13 mg/mL, resp. Emulsion and suspension concentrate, wettable powder and H2O-dispersible granule formulations containing III were given.

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	28.28	449.59

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-4.16	-4.16

STN INTERNATIONAL LOGOFF AT 17:06:23 ON 22 APR 2004

Welcome to STN International! Enter x:x

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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

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NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	JAN 27	Source of Registration (SR) information in REGISTRY updated and searchable
NEWS	4	JAN 27	A new search aid, the Company Name Thesaurus, available in CA/CAplus
NEWS	5	FEB 05	German (DE) application and patent publication number format changes
NEWS	6	MAR 03	MEDLINE and LMEDLINE reloaded
NEWS	7	MAR 03	MEDLINE file segment of TOXCENTER reloaded
NEWS	8	MAR 03	FRANCEPAT now available on STN
NEWS	9	MAR 29	Pharmaceutical Substances (PS) now available on STN
NEWS	10	MAR 29	WPIFV now available on STN
NEWS	11	MAR 29	No connect hour charges in WPIFV until May 1, 2004
NEWS	12	MAR 29	New monthly current-awareness alert (SDI) frequency in RAPRA

NEWS EXPRESS	MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 13 APRIL 2004
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

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* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 17:11:36 ON 22 APR 2004

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FULL ESTIMATED COST	0.21	0.21

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STRUCTURE FILE UPDATES: 21 APR 2004 HIGHEST RN 676437-01-7
DICTIONARY FILE UPDATES: 21 APR 2004 HIGHEST RN 676437-01-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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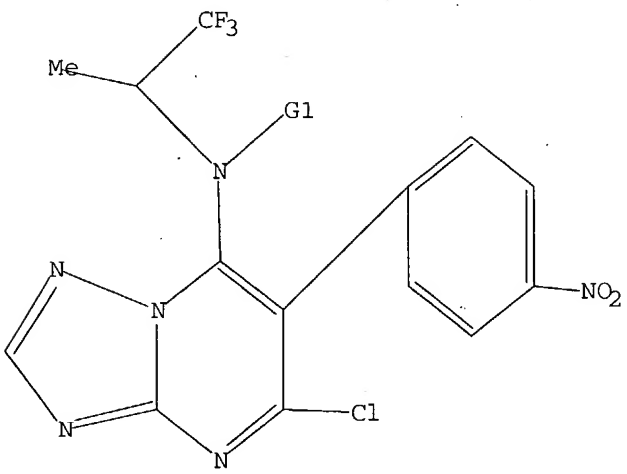

G1 H,Ak
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G4 X,Ak

Structure attributes must be viewed using STN Express query preparation.

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FULL SCREEN SEARCH COMPLETED - 367 TO ITERATE

100.0% PROCESSED 367 ITERATIONS 1 ANSWERS
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FULL ESTIMATED COST	155.42	155.63

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FILE CONTENT: 1988-PRESENT (VOL 140 ISS 16)(20040416/ED)

MOST RECENT CITATIONS FOR PATENTS FROM FIVE MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US 6706759 16 MAR 2004
DE 10335606 11 MAR 2004
EP 1396268 10 MAR 2004
JP 2004095205 25 MAR 2004
WO 2004022766 18 MAR 2004

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

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L3 4 SEA SSS FUL L1

=> file caol;d

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FILE 'CAOLD' ENTERED AT 17:12:39 ON 22 APR 2004
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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts

printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

YOU HAVE REQUESTED DATA FROM FILE 'MARPAT' - CONTINUE? (Y)/N:end

=> file caold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.42	265.47

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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

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Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 17:13:02 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 367 TO ITERATE

100.0% PROCESSED 367 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

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L5 0 L4

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION

FULL ESTIMATED COST 0.42 421.73

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FILE COVERS 1907 - 22 Apr 2004 VOL 140 ISS 17
FILE LAST UPDATED: 21 Apr 2004 (20040421/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L6   ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2004 ACS on STN
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AN 2001:195201 CAPLUS
DN 134:233069
TI Preparation of optically active fungicidal trifluoromethylalkylamino-triazolopyrimidines
IN Pfrengle, Waldemar; Pees, Klaus-Juergen; Albert, Guido; Carter, Paul; Rehnig, Annerose; Cotter, Henry Van Tuyl
PA American Cyanamid Co., USA
SO U.S., 11 pp., Cont.-in-part of U.S. 5,986,135.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 2

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	US 5986135	A	19991116	US 1998-160894	19980925

PATENT FAMILY INFORMATION:
FAN 1999:733059

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PI	US 5986135	A	19991116	US 1998-160894	19980925
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	JP 2000119275	A2	20000425	JP 1999-265647	19990920
				US 1998-160894 A	19980925
	KR 2000023437	A	20000425	KR 1999-41162	19990922
				US 1998-160894 A	19980925
	EP 989130	A1	20000329	EP 1999-307522	19990923
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OS MARPAT 134:233069
IT **329911-44-6P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of fungicidal optically active enantiomers of)
RN 329911-44-6 CAPLUS
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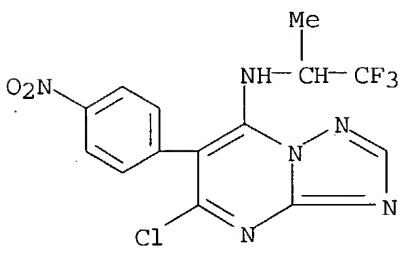

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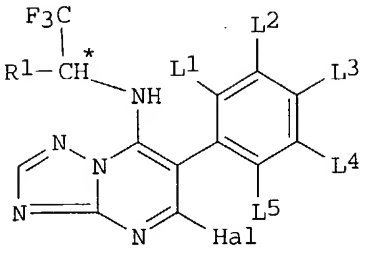

I

AB Optically active 7-(1,1,1-trifluoroalk-2-ylamino)-triazolopyrimidines I (R1 = C2-C6 alkyl; CH* = chiral carbon atom; Hal = halo; L1-L5 = H, halo, alkyl, alkoxy, or nitro), characterized in that the enantiomeric excess of the (S)-enantiomer is at least 70%, are prepared and show enhanced selective fungicidal activity against phytopathogenic fungi. The new compds. are processed with carriers, and optionally with adjuvants, to form fungicidal compns.

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L7 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:31452 CAPLUS
DN **136:96032**
TI Substituted triazolopyrimidines as anticancer agents
IN Schmitt, Mark R.; Kirsch, Donald R.; Harris, Jane E.; Beyer, Carl F.; Pees, Klaus-Juergen; Carter, Paul; Pfrengle, Waldemar; Albert, Guido
PA American Home Products Corporation, USA
SO PCT Int. Appl., 405 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

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				WO 2001-US20672W	20010628
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			US 2000-215585PP	20000630
			WO 2001-US20672W	20010628
JP 2004502691	T2	20040129	JP 2002-507815	20010628
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			WO 2001-US20672W	20010628
US 2002068744	A1	20020606	US 2001-895975	20010629
			US 2000-215585PP	20000630
NO 2002006195	A	20030227	NO 2002-6195	20021223
			US 2000-215585PP	20000630
			WO 2001-US20672W	20010628

OS MARPAT 136:96032

AB A method is provided for treating or inhibiting the growth of cancerous tumor cells and associated diseases in a mammal in need thereof which comprises administering to the mammal an effective amount of a substituted triazolopyrimidine derivative or a pharmaceutically acceptable salt thereof. Also provided is a method for treating or inhibiting the growth of cancerous tumor cells and associated diseases in a mammal in need thereof by interacting with tubulin and microtubules and promoting microtubule polymerization which comprises administering to the mammal an effective amount of a substituted triazolopyrimidine derivative or a pharmaceutically acceptable salt thereof.

L7 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2001:480706 CAPLUS

DN **135:61350**

TI Preparation of 5-halo-6-phenyl-7-N-(2,2,2-trifluoroethylamino)-1,2,4-triazolo[1,5-a]pyrimidine agrochemical fungicides

IN Pees, Klaus-Juergen; Krummel, Guenter; Cotter, Henry Van Tuyl; Albert, Guido; Rehnig, Annerose; May, Leslie; Pfrengle, Waldemar

PA American Cyanamid Co., USA

SO U.S., 6 pp.
CODEN: USXXAM

DT Patent

LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6255309	B1	20010703	US 1999-272916	19990319
	US 2003055069	A1	20030320	US 2001-840488	20010423
				US 1997-43820P P	19970414
				US 1999-272916 A3	19990319

PATENT FAMILY INFORMATION:

FAN 1999:571812

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5948783	A	19990907	US 1998-54580	19980403
				US 1997-43820P P	19970414

OS CASREACT 135:61350; MARPAT 135:61350

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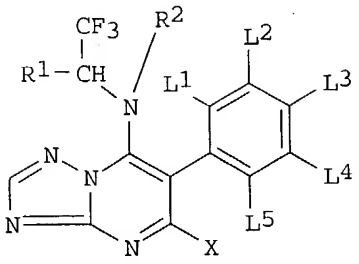

I

AB The title compds. (I; R1 = hydrogen, methyl; R2 = hydrogen, C1-10 alkyl; X = halogen; L1-L5 = hydrogen, halogen, alkyl, alkoxy; nitro; provided that at least one of L1-L5 = nitro or alkoxy, and further provided that when L3 = alkoxy then L2 and L4 ≠ hydrogen), useful as agrochem. fungicides (no data), are prepared Thus, 2,2,2-trifluoroethylamine was reacted with 5,7-dichloro-6-(4-methoxyphenyl)-1,2,4-triazolo[1,5-a]pyrimidine, forming 5-Chloro-6-(4-methoxyphenyl)-7-N-(2,2,2-trifluoroethylamino)-1,2,4-triazolo[1,5-a]pyrimidine, m.p. 183-185°.

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:195201 CAPLUS
DN **134:233069**
TI Preparation of optically active fungicidal trifluoromethylalkylamino-triazolopyrimidines
IN Pfrengle, Waldemar; Pees, Klaus-Juergen; Albert, Guido; Carter, Paul; Rehnig, Annerose; Cotter, Henry Van Tuyl
PA American Cyanamid Co., USA
SO U.S., 11 pp., Cont.-in-part of U.S. 5,986,135.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6204269	B1	20010320	US 1999-406574	19990924
				US 1998-160894 A2	19980925
	US 5986135	A	19991116	US 1998-160894	19980925

PATENT FAMILY INFORMATION:
FAN 1999:733059

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5986135	A	19991116	US 1998-160894	19980925
	ZA 9905673	A	20000330	ZA 1999-5673	19990902
				US 1998-160894 A	19980925
	JP 2000119275	A2	20000425	JP 1999-265647	19990920
				US 1998-160894 A	19980925
	KR 2000023437	A	20000425	KR 1999-41162	19990922
				US 1998-160894 A	19980925
	EP 989130	A1	20000329	EP 1999-307522	19990923
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
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	BR 9904354	A	20000912	BR 1999-4354	19990923
				US 1998-160894 A	19980925

CN 1250052	A	20000412	CN 1999-120740	19990924
			US 1998-160894 A	19980925
US 6204269	B1	20010320	US 1999-406574	19990924
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OS MARPAT 134:233069
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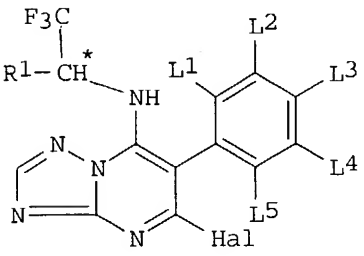

I

AB Optically active 7-(1,1,1-trifluoroalk-2-ylamino)-triazolopyrimidines I (R1 = C2-C6 alkyl; CH* = chiral carbon atom; Hal = halo; L1-L5 = H, halo, alkyl, alkoxy, or nitro), characterized in that the enantiomeric excess of the (S)-enantiomer is at least 70%, are prepared and show enhanced selective fungicidal activity against phytopathogenic fungi. The new compds. are processed with carriers, and optionally with adjuvants, to form fungicidal compns.

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:708827 CAPLUS
DN **129:302657**
TI Preparation of fungicidal [trifluoromethyl(alkyl)amino]triazolopyrimidines
IN Pees, Klaus-Juergen; Krummel, Guenter; Van Tuyl Cotter, Henry; Rehnig, Annerose; May, Leslie; Pfrengle, Waldemar; Albert, Guido
PA American Cyanamid Co., USA
SO PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9846608	A1	19981022	WO 1998-US5615	19980323
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				US 1997-843323 A	19970414
				US 1998-150572 A	19980910
	TW 460476	B	20011021	TW 1998-87103847	19980316
				US 1997-843323 A	19970414
	AU 9868671	A1	19981111	AU 1998-68671	19980323

AU 735730	B2	20010712	
			US 1997-843323 A 19970414
			WO 1998-US5615 W 19980323
EP 975635	A1	20000202	EP 1998-914274 19980323
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			WO 1998-US5615 W 19980323
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			US 1997-843323 A 19970414
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CN 1104433	B	20030402	CN 1998-805241 19980323
			US 1997-843323 A 19970414
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			US 1997-843323 A 19970414
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IL 132238	A1	20030529	IL 1998-132238 19980323
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PT 975635	T	20030930	PT 1998-914274 19980323
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CZ 292819	B6	20031217	CZ 1999-3596 19980323
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ZA 9803054	A	19991011	ZA 1998-3054 19980409
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EP 945453	A1	19990929	EP 1999-301910 19990312
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PATENT FAMILY INFORMATION:
FAN  1999:626195
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PI   WO 9948893         A1   19990930          WO 1999-US5915   19990319
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			US 1997-843323 A 19970414
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			WO 1998-US5615 A 19980323
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			WO 1999-US5915 W 19990319
BR 9909009	A	20001128	BR 1999-9009 19990319
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			WO 1999-US5915 W 19990319
JP 2003522100	T2	20030722	JP 2000-537876 19990319
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OS MARPAT 129:302657
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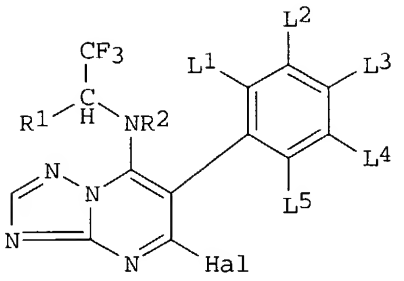

I

AB The title compds. [I; R1, R2 = H, (un)substituted alk(en)yl, alkynyl, alkadienyl or Ph; Hal = halo; L1-L5 = H, halo, alkyl, alkoxy, NO2], fungicides with selective activity, were prepared by amination of 5,7-dihalo-6-phenyltriazolopyrimidines with trifluoroalkylamines. The new compds. are processed with carriers and adjuvants to fungicidal compns. For example, a stirred mixture of 1.4 mmol 5,7-dichloro-6-(2-chloro-6-fluorophenyl)-1,2,4-triazolo[1.5a]pyrimidine with 30 mL CH2Cl2 was treated with a mixture of 4.2 mmol CF3CH2NH2 and 10 mL CH2Cl2 and the whole was stirred for 16 h at ambient temperature to give I (R2 = L2 = L3 = L4 = H, L5 = F) (II; R1 = H, L1 = Cl). II (R1 = Me, L1 = F) (III) inhibited mycelial growth of Alternaria solani and Rhizoctonia solani with MIC 0.78 and 3.13 mg/mL, resp. Emulsion and suspension concentrate, wettable powder and H2O-dispersible granule formulations containing III were given.

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L8          160 AMINO AND TRIAZOLOPYRIMIDINES

=> s l8 and  7-amino
L9           20 L8 AND  7-AMINO

=> s l8 and 4-halogens
L10           0 L8 AND 4-HALOGENS

=> s l8 and 5-halogens
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=> s l8 and 6-phenyl
L12           3 L8 AND 6-PHENYL

=> s l8 and 6-aryl
L13           0 L8 AND 6-ARYL

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The following are valid formats:

ABS --------- GI and AB
ALL --------- BIB, AB, IND, RE
APPS -------- AI, PRAI
BIB --------- AN, plus Bibliographic Data and PI table (default)
CAN --------- List of CA abstract numbers without answer numbers
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CBIB -------- AN, plus Compressed Bibliographic Data
DALL -------- ALL, delimited (end of each field identified)
DMAX -------- MAX, delimited for post-processing
FAM --------- AN, PI and PRAI in table, plus Patent Family data
FBIB -------- AN, BIB, plus Patent FAM
IND --------- Indexing data
IPC --------- International Patent Classifications
MAX --------- ALL, plus Patent FAM, RE
PATS -------- PI, SO
SAM --------- CC, SX, TI, ST, IT
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STD --------- BIB, IPC, and NCL

IABS -------- ABS, indented with text labels
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IMAX -------- MAX, indented with text labels
ISTD -------- STD, indented with text labels

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

HIT --------- Fields containing hit terms
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HITRN ------- HIT RN and its text modification
HITSTR ------ HIT RN, its text modification, its CA index name, and
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HITSEQ ------ HIT RN, its text modification, its CA index name, its
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FHITSTR ----- First HIT RN, its text modification, its CA index name, and
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FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
KWIC -------- Hit term plus 20 words on either side
OCC --------- Number of occurrence of hit term and field in which it occurs

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an arrow prompt (=>).  Examples of formats include: TI; TI,AU; BIB,ST;
TI,IND; TI,SO.  You may specify the format fields in any order and the
information will be displayed in the same order as the format
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L12           3 S L8 AND 6-PHENYL
L13           0 S L8 AND 6-ARYL

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L9   ANSWER 1 OF 20  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   2003:76783  CAPLUS
DN   138:137323
TI   Substituted 6-(2-tolyl)-triazolo[1,5-a]pyrimidines as fungicides
IN   Tormo i Blasco, Jordi; Sauter, Hubert; Mueller, Bernd; Gewehr, Markus;
     Grammenos, Wassilios; Grote, Thomas; Gypser, Andreas; Rheinheimer,
     Joachim; Rose, Ingo; Schaefer, Peter; Schieweck, Frank; Rack, Michael;
     Ammermann, Eberhard; Strathmann, Siegfried; Lorenz, Gisela; Stierl,
     Reinhard
PA   BASF Aktiengesellschaft, Germany; et al.
SO   PCT Int. Appl., 49 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.        KIND  DATE           APPLICATION NO.   DATE
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PI   WO 2003008417      A1   20030130       WO 2002-EP7578    20020708
     WO 2003008417      C2   20031030
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             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
             TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
             CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
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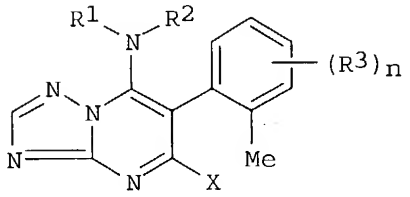
PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 2001-117402 A 20010718

OS MARPAT 138:137323

GI



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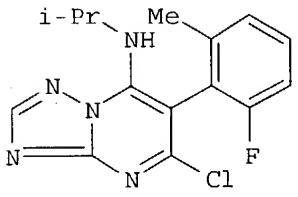


II

AB Title compds. I [R1-2 = H, alk(en/yn)yl, alkadienyl, etc.; R3 = halo, CN, alkyl, alkoxy, haloalkyl, etc.; n = 1-4; X = halo, CN, alkyl, alkoxy, etc.] are prepared For instance, 3-**amino**-1,2,4-triazole and di-Et (2-fluoro-6-methylphenyl)malonate (preparation given) are reacted (n-Bu3N, 180°, 6 h) and the intermediate treated with NaOH to give 5,7-dihydroxy-6-(2-fluoro-6-methylphenyl)-[1,2,4]triazolo[1,5-a]pyrimidine. This is converted to the dichloro derivative (POCl3, reflux, 8 h) and reacted with i-PrNH2 (Et3N, CH2Cl2) to yield II. Several example compds. at 63 ppm gave 97% control of Altenaria solani on tomato. I are useful for combating phytopathogenic fungi.

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:76781 CAPLUS
DN 138:137321
TI Preparation of 6-(2,6-difluorophenyl)-triazolo[1,5-a]pyrimidines as fungicides
IN Tormo i Blasco, Jordi; Sauter, Hubert; Mueller, Bernd; Gewehr, Markus; Grammenos, Wassilios; Grote, Thomas; Gypser, Andreas; Rheinheimer, Joachim; Rose, Ingo; Schaefer, Peter; Schieweck, Frank; Ammermann, Eberhard; Strathmann, Siegfried; Lorenz, Gisela; Stierl, Reinhard
PA BASF Aktiengesellschaft, Germany; et al.
SO PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003008415	A1	20030130	WO 2002-EP7575	20020708

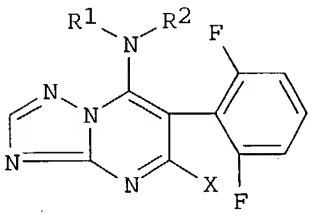
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,

NE, SN, TD, TG

EP 2001-117404 A 20010718

OS MARPAT 138:137321
GI



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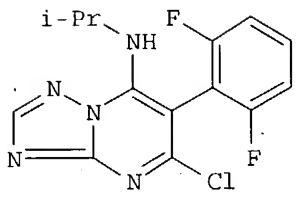
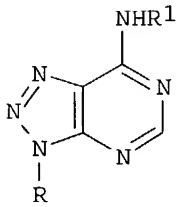


II

AB Title compds. I [R1-2 = H, alk(en/yn)yl, alkadienyl, etc.; X = halo, CN, alkyl, alkoxy, etc.] are prepared For instance, 3-**amino**-1,2,4-triazole and di-Et (2,6-difluorophenyl)malonate are reacted (n-Bu3N, 180°, 6 h) and the intermediate treated with NaOH to give 5,7-dihydroxy-6-(2,6-difluorophenyl)-[1,2,4]triazolo[1,5-a]pyrimidine. This is converted to the dichloro derivative (POCl3, reflux, 8 h) and reacted with i-PrNH2 (Et3N, CH2Cl2) to yield II. Several example compds. at 250 ppm gave 99% control of Altenaria solani on tomato. I are useful for combating phytopathogenic fungi.

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:88085 CAPLUS
DN 128:110380
TI Novel 3-Aralkyl-7-(**amino**-substituted)-1,2,3-triazolo[4,5-d]pyrimidines with High Affinity toward A1 Adenosine Receptors
AU Betti, Laura; Biagi, Giuliana; Giannaccini, Gino; Giorgi, Irene; Livi, Oreste; Lucacchini, Antonio; Manera, Clementina; Scartoni, Valerio
CS Dipartimento di Scienze Farmaceutiche, Facolta di Farmacia Universita di Pisa, Pisa, 56126, Italy
SO Journal of Medicinal Chemistry (1998), 41(5), 668-673
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
GI



I

AB Three series of several 1,2,3-triazolo[4,5-d]pyrimidine derivs. I (R = PhCH2, PhCH2CH2, 2-ClC6H4CH2; R1 = cyclohexyl, cyclopentyl, 3-methylcyclohexyl, p-tolyl, m-tolyl, α-methylbenyl, etc.) bearing various **amino** substituents at the 7 position and one of three lipophilic substituents at the 3 position were prepared starting from the corresponding 7-chloro compds., by nucleophilic substitution by the appropriate amine. Radioligand binding assays at bovine brain adenosine A1 and A2A receptors showed that some compds. possessed a high affinity and selectivity for the A1 receptor subtype. In particular the biol. results suggested the compds. I (R = cycloalkylamino, aralkylamino) were the most active derivs. The best lipophilic substituent R1 was 2-ClC6H4CH2, (A1 affinity Ki < 50 nM) followed by CH2Ph and CH2CH2Ph. This pattern of structure-activity relationship (SAR) was similar to that previously reported for analogous 1,2,3-triazolopyridazino derivs. [G. Biagi et al. (1994, 1995, 1996)] except for the compds. bearing substituted aromatic amines which presented a generalized and strong decrease of the A1 receptor affinity. These facts allowed us to attribute to these mols. a binding mode within the A1 adenosine receptor analogous to that of the corresponding triazolopyridazines.

RE.CNT 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

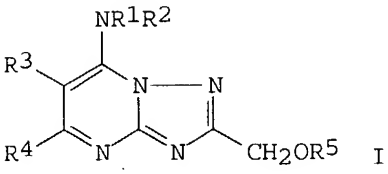
L9 ANSWER 4 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:501732 CAPLUS
DN 125:221428
TI Palladium-Catalyzed Allylic Coupling of 1,2,3-Triazolo[4,5-d]pyrimidines (8-Azapurines)
AU Konkel, Michael J.; Vince, Robert
CS College of Pharmacy, University of Minnesota, Minneapolis, MN, 55455-0343, USA
SO Journal of Organic Chemistry (1996), 61(18), 6199-6204
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
OS CASREACT 125:221428
AB The palladium-catalyzed coupling of the sodium salt of 7-**amino**-1,2,3-triazolo[4,5-d]pyrimidine (8-azaadenine) with allylic phosphates or carbonates resulted in mixts. of 2- and 3-substituted 1,2,3-**triazolopyrimidines**, which were separated by chromatog. 1-Substituted **triazolopyrimidines** were not isolated from these reactions. Regioselectivity (and stereoselectivity) was also observed for substitution of the allylic moiety when more than one isomer is possible from the reaction. The use of 5-**amino**-1,2,3-triazolo[4,5-d]pyrimidin-7-ones (8-azaguanine), instead of 8-azaadenine, also resulted in mixts. Alternate syntheses of the 3-allyl-1,2,3-triazolo[4,5-d]pyrimidines confirmed the structures of these compds.

L9 ANSWER 5 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1991:81809 CAPLUS
DN 114:81809
TI Preparation of **7-amino**-2-(hydroxymethyl)-s-triazolo[1,5-a]pyrimidine derivatives as cardiovascular agents
IN Shimizu, Shinichiro
PA Japan
SO Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF

DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 02212488	A2	19900823	JP 1989-32929	19890213
				JP 1989-32929	19890213

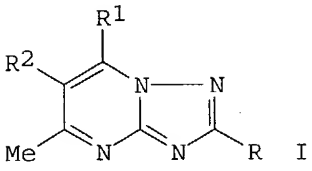
OS MARPAT 114:81809
GI



I

AB The title derivs. I (R1, R2 =H, lower alkyl, aralkyl; R3 = H, lower alkyl; R4 = H, lower alkyl, CF3; R3R4 may be alkylene; R5 = H, NO2, ester residue of organic carboxylic acids, CONR6R7; R6, R7 = H, lower alkyl) are prepared as drugs for treatment of cardiovascular disorders, especially cerebral ischemic diseases such as arteriosclerosis, cerebral and myocardial infarction, senile dementia, hyperlipemia, etc. I show coronary vasodilatory activity, inhibition on synthesis of prostaglandins and thromboxane A2, and hypolipemic activity. I are also useful as inhibitors for tumor metastasis, ulcer inhibitors, drugs for skin diseases, and hair growth. A DMF solution of 160 g 2-(hydroxymethyl)-5-methyl-s-triazolo[1,5-a]-pyrimidin-7-ol was treated with Ac2O and p-MeC6H4SO3H at 70° for 22 h to give 120 g 2-(acetoxymethyl)-5-methyl-s-triazolo[1,5-a]pyrimidin-7-ol, 60 g of which was further treated with a reaction mixture of POCl3 and PhNMe2 at 50-60° for 1 h to give 63 g 2-(acetoxymethyl)-5-methyl-7-chloro-s-triazolo[1,5-a]pyrimidine (II). Et2NH was added dropwise to an EtOH suspension of 24 g II at 0° over 15 min and the reaction mixture was further stirred at room temperature for 1 h to give 25 g I (R1 = R2 = Et, R3 = H, R4 = Me, R5 = Ac).

L9 ANSWER 6 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:571979 CAPLUS
DN 113:171979
TI 1,2,4-Triazolo[1,5a]pyrimidine. 5. Preparation of 7-**amino**-substituted 6-nitro-1,2,4-triazolo[1,5a]pyrimidine
AU Hempel, Ute; Lippmann, Eberhard; Tenor, Ernst
CS Sekt. Chem., Karl-Marx-Univ., Leipzig, DDR-7010, Ger. Dem. Rep.
SO Zeitschrift fuer Chemie (1990), 30(5), 170
CODEN: ZECEAL; ISSN: 0044-2402
DT Journal
LA German
OS CASREACT 113:171979
GI



I

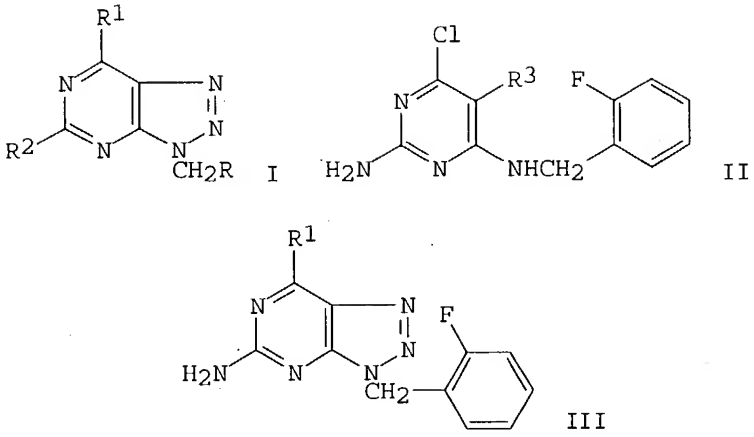
AB Nitration of **triazolopyrimidines** I (R = H, Me, R1 = OH, R2 = H) gave I (R2 = NO2) which on chlorination with POCl3 in PhNMe2 gave I (R = H, Me, R1 = Cl, R2 = NO2) along with side products I (R = H, Me, R1 = 4-Me2NC6H4, R2 = NO2). Reaction of I (R = H, Me, R1 = Cl, R2 = NO2) with primary and sec. amines gave 40% title compds. I (R = H, Me, R2 = substituted **amino**, R2 = NO2).

L9 ANSWER 7 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1989:114860 CAPLUS
DN 110:114860
TI Preparation of **7-amino**-3-benzyl-3H-1,2,3-triazolo[4,5-d]pyrimidines as anticonvulsants
IN Meier, Rene
PA Ciba-Geigy A.-G., Switz.
SO Eur. Pat. Appl., 28 pp.
CODEN: EPXXDW
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 288431	A1	19881026	EP 1988-810212	19880330
	EP 288431	B1	19920819		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
				CH 1987-1333	19870407
	AT 79624	E	19920915	AT 1988-810212	19880330
				CH 1987-1333	19870407
				EP 1988-810212	19880330
	ES 2051886	T3	19940701	ES 1988-810212	19880330
				CH 1987-1333	19870407
	IL 85947	A1	19930610	IL 1988-85947	19880331
				CH 1987-1333	19870407
	ZA 8802375	A	19891129	ZA 1988-2375	19880405
				CH 1987-1333	19870407
	DD 281190	A5	19900801	DD 1988-314431	19880405
				CH 1987-1333	19870407
	DK 8801843	A	19881008	DK 1988-1843	19880406
	DK 167681	B1	19931206		
				CH 1987-1333	19870407
	FI 8801582	A	19881008	FI 1988-1582	19880406
	FI 89359	B	19930615		
	FI 89359	C	19930927		
				CH 1987-1333	19870407
	NO 8801466	A	19881010	NO 1988-1466	19880406
	NO 167919	B	19910916		
	NO 167919	C	19911227		
				CH 1987-1333	19870407
	AU 8814302	A1	19881013	AU 1988-14302	19880406
	AU 616880	B2	19911114		

				CH 1987-1333	19870407
	JP 63258881	A2	19881026	JP 1988-83212	19880406
				CH 1987-1333	19870407
	HU 47577	A2	19890328	HU 1988-1714	19880406
	HU 206116	B	19920828		
				CH 1987-1333	19870407
	US 5204353	A	19930420	US 1991-814216	19911220
				CH 1987-1333	19870407
				US 1988-173840	19880328
				US 1989-376793	19890707
				US 1990-622304	19901205

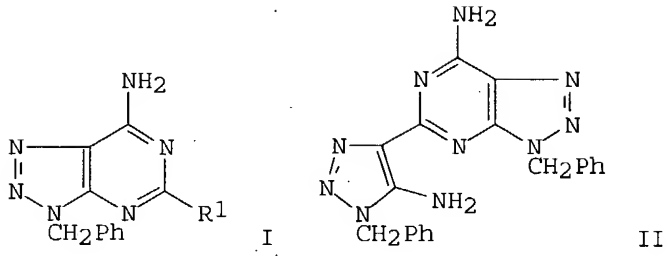
OS MARPAT 110:114860
GI



AB The title compds. (I; R = halophenyl, alkylphenyl, trifluoromethylphenyl, cyanophenyl; R1 = NH2, **amino** substituted with an acyl, aliphatic, cycloaliph., or cycloaliphaticaliph. group; R2 = H, alkyl, R1) were prepared 2-**Amino**-4,6-dichloropyrimidine was refluxed 20 h with 2-FC6H4CH2NH2 in EtOH containing Et3N to give benzylaminopyrimidine II (R3 = H) which was converted in 2 steps to II (R3 = NH2). The latter was stirred 2 h with NaNO2 in 25% HOAc to give triazolopyrimidine III (R1 = Cl) which was stirred 2 h with Me2NH in EtOH to give III (R1 = NMe2). I protect mice and rats against electroshock-induced convulsions at .apprx.3 mg/kg orally. A formulation of 10,000 tablets were prepared containing I (R = 2-FC6H4, R1 = NHMe, R2 = H) 500.0, lactose 500.0, starch 352.0, gelatin 8.0, talc 60.0, Mg stearate 10.0, and silica 20.0 g.

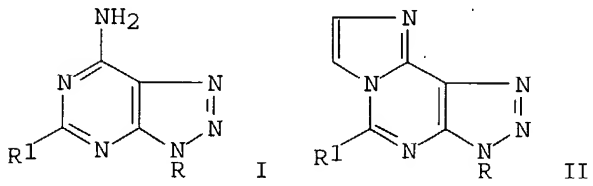
L9 ANSWER 8 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1988:75339 CAPLUS
DN 108:75339
TI One pot synthesis of 2,9-disubstituted 8-azaadenines (3,5-disubstituted **7-amino**-3H-1,2,3-triazolo[4,5-d]pyrimidines)
AU Barili, Pier Luigi; Biagi, Giuliana; Livi, Oreste; Mucci, Luciana; Scartoni, Valerio
CS Ist. Chim. Org., Univ. Pisa, Pisa, 56100, Italy
SO Journal of Heterocyclic Chemistry (1987), 24(4), 997-1001
CODEN: JHTCAD; ISSN: 0022-152X

DT Journal
LA English
OS CASREACT 108:75339
GI



AB Malononitrile was treated with PhCH2N3, R1CN (R1 = alkyl, Ph, tolyl, ClC6H4, pyridyl), and NaOEt to give **triazolopyrimidines** I. I were accompanied by dimer II in most reactions.

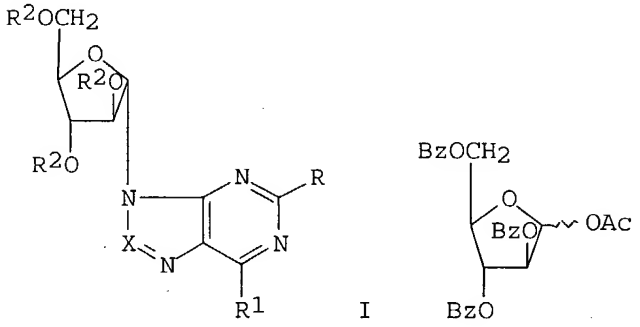
L9 ANSWER 9 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1977:468282 CAPLUS
DN 87:68282
TI Synthesis of some imidazo[1,2-c][1,2,3]triazolo[4,5-e]pyrimidines
AU Sugimoto, Takashi; Matsuura, Sadao
CS Coll. Gen. Educ., Nagoya Univ., Nagoya, Japan
SO Bulletin of the Chemical Society of Japan (1977), 50(5), 1359-60
CODEN: BCSJA8; ISSN: 0009-2673
DT Journal
LA English
OS CASREACT 87:68282
GI



AB The reaction of **7-amino**[1,2,3]triazolo[4,5-d]pyrimidine (I, R = R1 = H) with ClCH2CHO gave imidazo[1,2-c][1,2,3]triazolo[4,5-e]pyrimidine (II, R = R1 = H), which underwent facile ring opening in dilute HCl. II (R = H, R1 = Me; R = Me, R1 = H, Me) were similarly made from the appropriate I and ClCH2CHO.

L9 ANSWER 10 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1976:524283 CAPLUS
DN 85:124283
TI 1-O-Acetyl-2,3,5-tri-O-benzoyl-D-arabinofuranose and its use in glycosylation by fusion
AU Tolman, Richard L.; Baker, Donald A.
CS ICN Nucleic Acid Res. Inst., ICN Pharm., Irvine, CA, USA

SO Methods in Carbohydrate Chemistry (1976), 7, 59-62
CODEN: MCACAI; ISSN: 0097-3602
DT Journal
LA English
GI



I

II

AB α-D-arabinofuranosyl nucleosides I (X = CH, N; R,R' = H, Cl, NH2; R2 = H, Bz) were prepared from II by fusion with purine derivs. II was prepared by acetolysis of Me tri-O-benzoyl-α-D-arabinofuranoside. Thus, II and 2,6-dichloropurine were fused at 190° for 15 min to give 75% I (X = CH; R = R' = Cl; R2 = Bz) followed by debenzoylation and amination with MeOH and NH3 for 6 days to give 60% I (X = CH; R = Cl; R1 = NH2; R2 = H). Similarly prepared was **7-amino**-3-α-D-arabinofuranosyl-v-triazolo[4,5-d]pyrimidine.

L9 ANSWER 11 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1972:430142 CAPLUS
DN 77:30142
TI Syntheses of triazolopyrimidine derivatives from amitrole and their biological activity
AU Okabe, Takayuki; Taniguchi, Eiji; Maekawa, Kazuyuki
CS Fac. Agric., Kyushu Univ., Fukuoka, Japan
SO Gakugei Zasshi - Kyushu Daigaku Nogakubu (1972), 26(1-4), 105-15
CODEN: KNGZA2; ISSN: 0368-6264
DT Journal
LA English
AB Amitrole (3-**amino**-1,2,4-triazole) (I) [61-82-5] was condensed with active methylene ketones such as Et cyanoacetate, acetylacetone, ethyl acetoacetate to give the corresponding **7-amino**-5-hydroxy-s-triazolo[1,5-a]pyrimidine [35186-69-7], 5,7-dimethyl-s-triazolo[1,5-a]pyrimidine [7681-99-4], and 7-hydroxy-5-methyl-s-triazolo[1,5-a]pyrimidine (II) [2503-56-2]; from II some 5-methyl-7-substituted-s-**triazolopyrimidines** were synthesized and tested for herbicidal and fungicidal activity. 7-Chloro-5-methyl-s-triazolo[1,5-a]pyrimidine (III) [24415-66-5] synthesized from II plus POCl3, as well as 5-methyl-7-thiocyano-s-triazolo[1,5-a]pyrimidine (IV) [35186-71-1] prepared from III plus NH4SCN actively inhibited spore germination of Ophiobolus miyabeanus. IV showed antibiotic effects on Bacillus subtilis, Pellicularia filamentosa, [Rhizoctonia solani], and Phytophthora infestans and was herbicidally active on Atriplex gmelini, but showed no growth regulatory activity on rice.

L9 ANSWER 12 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1972:126928 CAPLUS
DN 76:126928
TI v-Triazolo[4,5-d]pyrimidines (8-azapurines). VIII. Synthesis, from 1,2,3-triazoles, of 1- and 2-methyl derivatives of 5,7-disubstituted v-triazolo[4,5-d]pyrimidines (7- and 8-methyl 2,6-disubstituted 8-azapurines)
AU Albert, Adrien; Taguchi, Hiroyasu
CS Dep. Med. Chem., John Curtin Sch. Med. Res., Canberra, Australia
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1972), (4), 449-56
CODEN: JCPRB4; ISSN: 0300-922X
DT Journal
LA English
GI For diagram(s), see printed CA Issue.
AB 4-**Amino**-1-methyl-1H-1,2,3-triazole-5-carboxamide was fused with thiourea to give 5-mercapto-1-methyl-1H-v-triazolo[4,5-d]pyrimidin-7(6H)-one (I) which was methylated and oxidized to give the 5-(methylsulfonyl) analog (II); this, when heated with NaOMe or NH3, gave the 5-methoxy and 5-**amino** compds. resp. 5-**Amino**-2-methyl-2H-1,2,3-triazole-4-carboxamide similarly gave, via the 5-mercapto compound (III), 5-(methylsulfonyl)-2-methyl-2H-v-triazolo[4,5-d]pyrimidin-7(6H)-one (IV), which was converted into the 5-methoxy, 5-ethoxy, 5-**amino** (V), 5-(methylamino), and 5-(dimethylamino) analogs; a by-product of the reaction of IV with MeNH2 was 5-**amino**-2-methyl-N-[bis(methylamino)methylene]-2H-1,2,3-triazole-4-carboxamide. Alkaline hydrolysis of II and IV gave the corresponding 5,7-diones; a by-product of the hydrolysis of II was u-methyl-4-ureido-1H-1,2,3-triazole-5-carboxylic acid. I and III was converted into the corresponding 5,7-bis(methylthio) compds., which gave **7-amino**-5-(methylthio) compds. on heating with NH3-EtOH. 5,7-Diamino compds. were prepared by heating the derived sulfones with NH3-EtOH; in contrast, treatment with NaOMe and aqueous alkali gave **7-amino**-5-methoxy and **7-amino**-5-oxo compds. resp. 5,7-Dichloro-2-methyl-2H-v-triazolo[4,5-d]pyrimidine, prepared from the appropriate 5,7-dione, gave the 5,7-diamine with NH3-EtOH. Ionization consts. and spectra of the compds. were recorded. V inhibited the Ehrlich ascites tumor and the Ridgeway osteogenic tumor in mice.

L9 ANSWER 13 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1972:10168 CAPLUS
DN 76:10168
TI Biotransformation of trapymin (Rocornal)
AU Pfeifer, S.; Mann, I.; Wierer, A.; Thomas, D.
CS Sekt. Chem., Humboldt-Univ. Berlin, Berlin, Fed. Rep. Ger.
SO Pharmazie (1971), 26(9), 549-54
CODEN: PHARAT; ISSN: 0031-7144
DT Journal
LA German
AB 5-Methyl-7-diethylamino-s-triazolo[1,5-a]pyrimidine (Rocornal)(I) [15421-84-8] administered i.p. to humans, rats, and rabbits, was dealkylated and appeared in the urine principally as 5-methyl-**7-amino**-s-triazolo[1,5-a]pyrimidine(II) [33376-96-4]. I was also excreted by humans unchanged and as the glucuronide.

L9 ANSWER 14 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1968:496777 CAPLUS
DN 69:96777
TI 5-Nitrofuran and 5-nitrothiophene derivatives

PA Boehringer, C. F., und Soehne G.m.b.H.
SO Brit., 4 pp.
CODEN: BRXXAA
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI GB 1123247		19680814		
			DE	19660618
DE 1670095			DE	
FR 1527537			FR	
US 3522256		19700000	US	

GI For diagram(s), see printed CA Issue.
AB Hydrazones are treated with oxidizing agents, hydrazinopyridazines are condensed, or amidrazones are treated with agents for splitting of elements of NH3 to yield 5-nitrofuran or 5-nitrothiophene derivs. with uninary antimicrobial activity. Thus, 6.65 g. 3-methyl-6-hydroxinopyridazine semihydrate was dissolved in 50 ml. dioxane and mixed at 50° with 7 g. 5-nitro-2-furfural. After 30 min., crystals were obtained on cooling and were filtered, and washed with dioxane and Et2O to give an 85% yield of 1-(5-nitro-2-furfurylidene)-2-(3-methyl-6-pyridazinyl)hydrazine (I), m. 242-3°. Concentrated HCl (.apprx.2 ml.) was added to 5.5 g. I in 700 ml. EtOH at the b.p. until a clear solution was obtained. A solution of 29 g. FeCl3.6H2O in 330 ml. EtOH was added, over 45 min., to the refluxing mixture and refluxing continued for 3 hrs. After overnight cooling, the solution was filtered, the residue washed with EtOH and recrystd. from 100 ml. 80% aqueous HCONMe2, in the presence of activated charcoal, at 110°, to give a 61.4% yield of 3-(5-nitro-2-furyl)-6-methyl-s-triazolo[4,3-b]pyridazine (Ia), m. 246-7°. Ia, m. 245-6°, was obtained by refluxing 1.2 g. 3-methyl-6-hydrazinopyridazine and 3.1 g. 5-nitrofuran-2-carboxylic acid in 5 ml. diethylene glycol for 1 hr., cooling, making alkaline, and extracting with CH2Cl2.
3-(5-Nitro-2-furyl)-s-triazolo[4,3-b]pyridazine (II), m. 280-3°, was similarly prepared from N-(3-pyridazinyl-**amino**)-5-nitro-2-furamidine and a 41% yield of II, m. 289-93°, was prepared from 1-(5-nitrofurfurylidene)-2-(3-pyridazinyl)-hydrazine-HCl. Other derivs. prepared were 3-(5-nitro-2-thienyl)-6-methyl-s-triazolo[4,3-b]pyridazine, and 3-(5-nitro-2-furyl)-**7-amino**-s-triazolo[4,3-b]pyridazine.

L9 ANSWER 15 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1968:476444 CAPLUS
DN 69:76444
TI Electronic properties of N-heteroaromatics. XXI. Polarographic behavior of v-triazolo[d]pyrimidine derivatives
AU Okano, Teisuke; Noji, Masahide
CS Tohoku Univ., Sendai, Japan
SO Yakugaku Zasshi (1968), 88(4), 434-8
CODEN: YKKZAJ; ISSN: 0031-6903
DT Journal
LA Japanese
AB Polarographic behavior of v-triazolo[d]pyrimidine (I) and its 5-**amino** (II), 7-**amino** (III), 5,7-diamino (IV), 7-**amino**-5-hydroxy (V), 5-**amino**-7-hydroxy (VI), 5,7-dihydroxy (VII), and 7-hydroxy (VIII) derivs. was investigated. While I to V were polarographically reducible, no reduction waves were obtained with

VI, VII, and VIII, indicating that substituents at 7-position have a dominant effect on reducibility. Substituents at 5-position had only a slight effect on reducibility. It was presumed from the substituent effect that the 1st step of reduction may take place at N6-C-7 double bond of the pyrimidine moiety. It was revealed that triazolopyrimidine derivs. were more easily reduced at the dropping Hg electrode than the corresponding purine derivs., which might be ascribable to the difference in tendencies of inflow of π-electrons into the pyrimidine ring moiety from the neighboring ring. Parallel relationship was found between the ease of reduction and energy levels of the lowest vacant orbitals, which have been computed by simple L.C.A.O.-M.O. method.

L9 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1964:3162 CAPLUS
DN 60:3162
OREF 60:523e-g
TI Condensed heterocycles. IV. Condensation of 3-**amino**-1,2,4-triazoles with diaceto- and dipropionitriles
AU Levin, Ya. A.; Kukhtin, V. A.
CS Cine-Photo Res. Inst., Kazan
SO Zhurnal Obshchei Khimii (1963), 33(8), 2678-82
CODEN: ZOKHA4; ISSN: 0044-460X
DT Journal
LA Unavailable
GI For diagram(s), see printed CA Issue.
AB Heating 3-**amino**-5-substituted 1,2,4-triazoles with substituted β-aminoacrylonitriles 30-40 min at 155-200° gave (Ia) (R, R', R'' % yield, and m.p. shown, resp.): H Me, H (I), 84, 246-7° (picrate decomposed 212-14°); Pr, Me, H, 61, 180-1°; C6H13, Me, H, 56, 128-30°; H, Et, Me (II), 72, 262-3°; Pr, Et, Me, 51, 225-6°. I refluxed with Ac2O in C5H5N gave the Ac derivative, m. 230°; similarly was prepared Ac derivative of II, m. 1402°, purified on Al2O3 in C6H6. I and tosyl chloride gave 75% ptoluenesulfonamido analog, decomposed 283-5° (λ 304 mμ). Treated with Br vapors at 60° in H2O, I gave 88% 4-imino-5bromo-6-methyt-1,2,4-triazolo[2,3-a]pyrimidine, decomposed 2457° (λ 261 and 298 mμ). I and aqueous I-KI in the presence of K2CO3 at 70-80° gave 4-**amino**-6-methyl-5-iodo-1,2,4-triazolo[2,3-a]pyrimidine, decomposed 233-5° (λ 260 and 300 mμ). 4-Chloro-5-hexyl-6-methyl-1,2,4-triazolo[2,3-a]pyrimidine, m. 412°, formed in 82% yield from the 4-oxo analog by refluxing in POCl3 3 hrs. Treated with NH3 in EtOH at 0°, then heated 3 hrs. in an ampul at 100°, this gave 83% 4-**amino**-5-hexyl-6methyl-1,2,4-triazolo[2,3-a]pyrimidine, m. 230-1°, which could not be prepared by the above condensation of aminotriazole with dipropionitrile even at 230°. I and concentrated HCl in 5 hrs. at 140° in a sealed tube gave 3-**amino**-1,2,4-triazole, isolated as the picrate, decomposed 228-30°. Ultraviolet spectra of Ia are shown.

L9 ANSWER 17 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1960:129047 CAPLUS
DN 54:129047
OREF 54:24761h-i,24762a-f
TI Pyrimidine derivatives. VII. 1,2,4-**Triazolopyrimidines**. 6
AU Shirakawa, Kenzo
CS Takeda Pharm. Inds., Ltd., Osaka
SO Yakugaku Zasshi (1960), 80, 952-6

CODEN: YKKZAJ; ISSN: 0031-6903
DT Journal
LA Unavailable

AB cf. CA 54, 11038e. 2-Hydrazino-4-hydroxy-5-ethoxycarbonylpyrimidine (1 g.) in 2 ml. HC(OEt)3 and 3 ml. BuOH refluxed 40 min., cooled, and the product filtered off and recrystd. (H2O) gave 0.75 g. 5-hydroxy-6-ethoxycarbonyl-1,2,4-triazolo[4,3-a]pyrimidine (I), m. 243-5° (decomposition). 5-**Amino**-1,2,4-triazole (II) (21 g.) and 54 g. EtOCH:C(CO2Et)2 in 40 ml. AcOH refluxed 3 hrs., 50 ml. H2O added, cooled, the product filtered off, this in 230 ml. 5% HCl heated, cooled, and the insol. portion collected gave 24.3 g. 6-ethoxycarbonyl-7-hydroxy-1,2,4-triazolo [2,3-a] pyrimidine (III), plates, m. 247° (decomposition) (H2O). I (0.2 g.) fused 5 min. at 200-5° and the product recrystd. (H2O) gave III. III (5 g.) in 20 ml. 20% HCl refluxed 20 min. and the product concentrated gave 2.8 g. 6-HO2C analog (IV) of III, m. 292° (decomposition) (H2O). IV (1 g.) heated 5 min. at 260° and the product recrystd. (H2O) gave 0.6 g. 7-hydroxy-1,2,4-triazolo[2,3-a]pyrimidine (V), m. 293° (decomposition). II (5 g.) and 10.5 g. EtOCH:C(CN)CO2Et (VI) in 30 ml. MeOCH2CH2OH refluxed 3 hrs. and the product filtered off gave 2 g. Et 2-cyano-3-(1,2,4-triazol-5-ylamino)acrylate (VII), m. 222° (80% AcOH). III (3 g.) and 13 g. POCl3 refluxed 2 hrs., the product concentrated, the residue with ice made alkaline with 30% NH4OH, and the precipitate filtered off gave 0.5 g. 6-ethoxycarbonyl-7-**amino**-1,2,4-triazolo [2,3-a] pyrimidine (VIII), plates, m. 218° (H2O). II (2.5 g.) and 5 g. VI in 30 ml. AcOH refluxed 8 hrs. and cooled gave 1.5 g. VIII. VII (2 g.) heated 2 min. at 220° and the product treated with NH4OH gave 0.5 g. VIII. PhCH:NNHC(:NH)NH2 (27 g.) and 29 g. VI in 300 ml. 99% EtOH refluxed 4 hrs. and the product filtered while hot and washed with EtOH gave 19.2 g. 2-benzylidenehydrazino-4-hydroxy-5-cyanopyrimidine (IX), leaves, m. 313° (decomposition) (HCOMe2-EtOH). IX (5.5 g.) in 6 ml 80% N2H4.H2O and 20 ml. H2O refluxed 5 min., the oily product removed by washing with C6H6, and the aqueous layer treated with HCl to pH 5 gave 2.7 g. 2-hydrazino-4-hydroxy-5-cyanopyrimidine (X), m. above 320°. X (5 g.) in 35 ml. 98% HCO2H refluxed 10 min. and the product recrystd. (H2O) gave 4.9 g. 5-hydroxy-6-cyano-1,2,4-triazolo[4,3-a]pyrimidine (XI), leaves, m. 258-9°. II (16.8 g.) in 8 g. NaOH, 24 g. H2O, and 80 ml. EtOH treated with 34 g. VI in 400 ml. EtOH, the mixture kept 6 hrs. at room temperature, refluxed 1 hr., the solution cooled at 0°, and the precipitate taken up in warm H2O and acidified with HCl gave 10.8 g. 6-cyano-7-hydroxy-1,2,4-triazolo[2,3-a]pyrimidine (XII), needles, m. 300-1° (decomposition). XI (1 g.) fused 4 min. and the product recrystd. (H2O) gave 0.6 g. XII. II (10 g.) and 16 g. EtOCH:C(CN)2 in 50 ml. AcOH refluxed 3 hrs. and the product filtered gave 3.7 g. 6-cyano-7-**amino**-1,2,4-triazolo[2,3-a]pyrimidine (XIII), needles, m. above 300° (70% HCO2H). XII (0.5 g.) added portionwise to 6 ml. 95% H2SO4 at 0°, the mixture kept overnight, 20 g. ice and concentrated NaOH added (to pH 3), and the product filtered gave 0.2 g. 6-carbamoyl-7-hydroxy-1,2,4-triazolo[2,3-a]pyrimidine (XIV), needles, m. 318-20° (decomposition) (90% AcOH). III (0.2 g.) in 10 ml. 30% NH4OH in a closed container kept 30 days at room temperature and the product concentrated gave 0.1 g. XIV. XIII (0.2 g.) added to 2 ml. 95% H2SO4 at 30°, kept overnight at 0%, and the product with ice made alkaline with NaOH and filtered off gave 0.1 g. 6-carbamoyl-7-**amino**-1,2,4-triazolo[2,3-a]pyrimidine (XV), m. above 300° (70% HCO2H).

VIII (1 g.) in 10 ml. 30% NH4OH kept 15 days at room temperature and the product filtered off gave 0.1 g. XV.

L9 ANSWER 18 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1958:88116 CAPLUS
DN 52:88116
OREF 52:15543i,15544a-i,15545a-i,15546a-e
TI Synthesis of the v-triazolo[d]pyrimidine analogs of adenosine, inosine, guanosine, and xanthosine, and a new synthesis of guanosine
AU Davoll, J.
CS Parke, Davis, & Co., Ltd., Hounslow, UK
SO Journal of the Chemical Society, Abstracts (1958) 1593-9
CODEN: JCSAAZ; ISSN: 0590-9791
DT Journal
LA Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. C.A. 46, 3959e. The title compds. and other glycosyl-v-triazolo[d]pyrimidine were synthesized from chloromercuri derivs. of appropriate **triazolopyrimidines** (I) prepared by modifications of standard methods, acetylated, and the AcO derivs. (II) converted into chloromercuri compds. (III) which were condensed with acylglycosyl halides as described for the corresponding purines (cf. Davoll and Lowy, C.A. 45, 10202d). AcOH (22 ml.) and 200 ml. aqueous 5,6-diamino-4-D-glucosylamino-2-methylthiopyrimidine, prepared according to Holland, et. al. (C.A. 43, 146c), from 6.5 g. 6-**amino**-4-D-glucosylamino-2-methylthiopyrimidine, were stirred with dropwise addition of 1.43 g. NaNO2 in 20 ml. H2O, the mixture was kept 2 hrs. at room temperature, the solution evaporated in vacuo below 40°, the residue acetylated with Ac2O-C5H5N at room temperature, the product (3.64 g.) extracted with CHCl3, the amorphous powder refluxed 2 hrs. in 250 ml. alc. containing Raney Ni (from 28 g. alloy), filtered hot and the filtrate and washings evaporated, the residue (1.77 g.) deacetylated with NH3 in MeOH at 0°, and the product converted into 1.41 g. picrate, m. 201° (decomposition after 4 recrystns. from H2O). Treatment of the picrate with Dowex Number 1 anion exchange resin gave I (R = H, R1 = NH2, R2 = β-D-glucopyranosyl) (Ia), m. 241° (decomposition) (H2O), [α]20D -22° (c 1.0, H2O). II in 10 vols. cold H2O solubilized by the addition of 1 or 2 equivs. of N NaOH, the filtered solution treated with 1 mole HgCl2 in hot alc. (8 ml./g. 20 vols. H2O, and 1.5 parts by weight (of I) Hyflo Supercel, the mixture cooled and filtered, and the residue washed, dried, and powdered gave 80-90% III. In the reaction of III with tetra-O-acetylglucosyl bromide the procedure of D. and L. (loc. cit.) was followed; reactions using tri-O-benzoyl-D-ribofuranosyl chloride (IV) were carried out according to Kissman, et al. (C.A. 49, 8298e), except that the final extraction of the crude condensation product with Et2O was omitted. The crude wet product from the nitrosation of 35 g. 4,6-diamino-2-mercaptopyrimidine refluxed 1 hr. with stirring with 3 l. H2O, 120 ml. NH4OH (d. 0.88), and Raney Ni (from 180 g. alloy) and the mixture filtered hot, evaporated in vacuo to 1.2 l. and shaken with C, the hot filtrate treated with 75 cc. AcOH and stirred with dropwise addition of 13 g. NaNO2 in 100 ml. H2O gave 13.5 g. I (R = R2 = H, R1 = NH2) (Ib). Ib (2 g.) and 20 ml. Ac2O refluxed 4 hrs. and the cooled mixture filtered, the residue washed with alc. and dried gave 2.06 g. acetamido compound, C6H6N6O, m. 293-4° (50% EtOCH2CH2OH). The corresponding IIIb (9.05 g.) and 10 g. tetra-o-acetyl-D-glucopyranosyl bromide gave 8.5 g. sirup, crystallized from 150 ml. alc. to give 0.5 g. needles, m. 270°, not giving a crystalline product on deacetylation with NH3 in MeOH. The alc.

filtrate evaporated and the residue deacetylated with NH3 in MeOH at 0° gave 0.85 g. (?) **7-amino**-1-β-D-glucopyranosyl-v-triazolo[d]pyrimidine (V) (R = H, R1 = NH, R2 = β-D-glucopyranosyl) (Va), C10H14N6O5, m. 250-1° (decomposition) (H2O); picrate, m. 160° (effervescence of 1 mole alc. of crystallization) (50% alc.). Addition of picric acid to the filtrate from Va gave 1.53 g. Ia picrate, converted to Ia with ultraviolet absorption spectrum identical with that of the above synthetic material. IIIb (16.7 g.) condensed with 1.09 moles IV, the sirup (24.5 g.) deacetylated with NaOMe, the mixture neutralized with CO2 and evaporated, the residue triturated with dry Et2O and the dried, BzOMe-free material crystallized from 125 ml. H2O and decolorized with C yielded 16% 8-azaadenosine (I, R = H, R1 = NH, R2 = 3-β-D-ribofuranosyl) (Ic), m. 218-19° (H2O), [α]22D -79° (c 0.46, H2O); picrate, m. 184° (decomposition) (H2O). Addition of picric acid to the mother liquor from Ic gave 7.25 g. impure picrate, converted to amorphous material, λ 273 mμ (0.1N HCl), λ 287 mμ (0.1N NaOH). Ic (2 g.) and 5 g. NaNO2 in 25 ml. hot H2O cooled rapidly, the solution treated with 5 ml. AcOH, kept 1 hr., diluted with 25 ml. H2O, stored 18 hrs., treated with aqueous Pb(OAc)2 and NH4OH, and filtered, the Pb salt taken up in 20% AcOH, the solution saturated with H2S, the filtered solution evaporated, and the residue (1.87 g.) repeatedly recrystd. (80% alc.) gave 1.38 g. 8-azainosine (I, R = H, R1 = HO, R2 = β-D-ribofuranosyl) (Id), C9H11N5O5, m. 199-200°, [α]21D -54° (c 1.78, H2O). NaNO2 (4.85 g.) in 30 ml. H2O added dropwise with stirring to 8.5 g. 2,4,6-triaminopyrimidine in 220 ml. 10% AcOH, the mixture kept 1 hr., diluted with 115 ml. AcOH, and hydrogenated 1 hr. with 5% Pd-C, the filtered solution treated dropwise with 4.85 g. NaNO2 in 30 ml. H2O with stirring and filtered, the product treated with C in hot dilute aqueous NH4OH, and the hot filtrate acidified with AcOH gave 7.55 g. I (R = R1 = NH, R2 = H) (Ie). Ie (9.76 g.) refluxed 30 min. in 98 ml. Ac2O, the cooled mixture filtered, the residue washed with alc., the triacetyl compound, m. 210° (decomposition), boiled with 200 ml. moist EtOC2H4OH and filtered and the residue washed with EtOH gave 9.94 g. diacetamido derivative, m. 280° (decomposition), converted to the chloromercuri compound (IIIe). IIIe (8 g.) and 1 mole IV condensed and the pale yellow glass (11.4 g.) deacylated with NaOMe yielded 42% (?) 5,7-diamino-β-D-ribofuranosyl-v-triazolo[d]pyrimidine(s) (VI), m. 127-50° (H2O). PhCH2MeNH (9 ml.) and 3 g. 2,4-diamino-6-chloropyrimidine refluxed 1 hr., the cooled mixture extracted with 60 ml. boiling EtOAc, the extract washed with 5% AcOH, and the dried (Na2SO4) extract evaporated gave 2.15 g. 2,4-diamino-6-(N-methylbenzylamino)pyrimidine acetate, m. 146-8°, which, nitrosated in 20% AcOH, the product hydrogenated in 50% AcOH with 10% Pd-C, and the filtered solution treated with 1 mole aqueous NaNO2 and filtered, gave I (R = R1 = NH, R2 = Me) (If), C5H7N7, m. 294-5° (H2O), insol. in alkali. IIIe and IV condensed and the crude product (18.9 g.) deacylated with NH3 in MeOH, treated with HNO2 and deacylated with NaOMe gave 1.26 g. (?) V (R = NH2, R1 = HO, R2 = β-D-ribofuranosyl) (Vb), C9H12N6O5, m. above 200° (decomposition), [α]20D -75° (c 0.9, H2O), hydrolyzed 2 hrs. in boiling N HCl to give material with the spectrum of I (R = NH2, R1 = HO, R2 = H). VI (0.45g.) refluxed 45 min. in 5 ml. Ac2O and the solution evaporated, the residue treated as above also gave 24% Vb, identified by ultraviolet spectra in acid and alkali. 2-Methylthio-9-β-D-ribofuranosyladenine (D. and L., loc. cit.) (0.5 g.) in 100 ml. 0.4N H2SO4 treated with 1.2 g. NaNO2 and the mixture kept 18 hrs., neutralized with

NH4OH and evaporated to 15 ml. gave 0.46 g. 2-methylthio-9-β-D-ribofuranosylhypoxanthine, (VII), m. 246° (decomposition). VII (0.5 g.) in 4 ml. aqueous NH4OH (d. 0.88) and 4 ml. alc. NH3 (saturated at 0°) heated 18 hrs. at 130-2° in a sealed tube, the cooled mixture evaporated and the residue recrystd. (H2O) 4 times with decolorizing C gave 0.12 g. authentic guanosine. NaNO2 (0.69 g.) in a min. of H2O added to 1.71 g. 4,5,6-triamino-2-methylthiopyrimidine in 55 ml. 10% AcOH and filtered, the precipitate treated with C in hot dilute aqueous NH4OH, and the filtered solution acidified with AcOH gave 1.55 g. I (R = MeS, R1 = NH, R2 = H), m. 282° (decomposition), refluxed (1 g.) 2 hrs. in 5 ml. Ac2O and the cooled mixture diluted with 10 ml. anhydrous Et2O to give 1.06 g. crystalline diacetyl compound, m. 153-5°, transformed on standing in the open with loss of 1 Ac group to give 7-acetamido-5-methylthio-v-triazolo[d]pyrimidine (Ig), m. 215-17°, recrystd. (70% alc.) to give solvated needles, C7H8N6OS.C2H6O, m. 219-220°, transformed to the corresponding chloromercuri compound (IIIg). IIIg (23 g.) and 1 mole IV condensed and the product (31 g.) deacylated with NaOMe, taken up in 175 ml. hot H2O and treated with C, the solution kept 1.5 hrs. at room temperature and filtered gave 3.79 g. I (R = MeS, R1 = NH2, R2 = β-D-ribofuranosyl) (Ih), m. 200-1° (H2O). The filtrate kept 20 hrs. at 3° and filtered gave 2.8 g. (?) V (R = MeS, R1 = NH2, R2 = β-D-ribofuranosyl) (Vc), m. 156-8° (H2O). Treatment of Ih with Ac2O-C5H5N at room temperature yielded 84% I (R = H, R1 = NH2, R2 = tri-O-acetyl-β-D-ribofuranosyl), m. 152-3° (alc.), boiled (0.14 g.) 2 hrs. in 10 ml. alc. with 1 g. Raney Ni and the product deacetylated with NH3 in MeOH to give 18 mg. Ic. Desulfurization of Vc gave an amorphous product producing gelatinous solns. in H2O, λ 285 mμ (0.1N HCl), 292 mμ (0.1N NaOH). Ih (0.5 g.) in 100 ml. N HNO3 treated 20 hrs. at room temperature with 1.2 g. NaNO2 and the mixture filtered gave 0.43 g. I (R = MeS, R1 = HO, R2 = β-D-ribofuranosyl) (Ii), m. 181-3° (sintering above 178°) (H2O). Ii (0.5 g.) aminated as above (preparation of guanosine) and the product isolated through the Pb salt yielded 8% 8-azaguanosine (I, R = NH, R1 = HO, R2 = β-D-ribofuranosyl) (Ij), C9H12N6O5, m. 250-2° (decomposition) (H2O), hydrolyzed 2 hrs. with boiling N HCl to give a compound with the ultraviolet absorption spectrum of 5-**amino**-7-hydroxy-v-triazolo[d]pyrimidine, λ 250 mμ (0.1N HCl). Vc (0.5 g.) and 1.2 g. NaNO2 in 12 ml. hot H2O and the rapidly cooled solution treated with 1.2 ml. AcOH, the mixture kept 24 hrs. and the product isolated through the Pb salt yielded 56% (?) V (R = MeS, R1 = HO, R1 = β-D-ribofuranosyl) (Vd), m. 214-15°. I (R = NH2, R1 = HO, R2 = H) (15.5 g.) refluxed 2 hrs. in 155 ml. Ac2O and the cooled mixture filtered, the product washed with alc. and dried gave 23.2 g. diacetyl derivative, m. 219°. The corresponding chloromercuri compound (31 g.) condensed with 1.15 moles IV, the pale yellow gum (41.5 g.) refluxed 1 hr. with NaOMe (from 2.5 g. Na in 400 ml. MeOH), the mixture evaporated, the residue in 500 ml. H2O made just acidic with AcOH, boiled and treated with C, the filtered solution kept 18 hrs. at room temperature and filtered gave 7.33 g. material, recrystd. to give 6.28 g. (?) 5-**amino**-7-hydroxy-2-β-D-ribofuranosyl-v-triazolo[d]pyrimidine (VIII), m. 230-5° (sintering) (H2O), [α]20D -79° (c 0.77, 0.1N NaOH). The filtrate evaporated to 200 ml. and cleared by heat, kept 5 hrs. and filtered yielded 4.62 g. material recrystd. (H2O) to give 3.9 g. Ij, [α]21D -97° (c 1.0, 0.1N NaOH). The mother liquors evaporated to

50 ml. gave 4.13 g. material containing 85% Ij, deaminated to yield pure I (R = R1 = HO, R2 = β-D-ribofuranosyl) (I-k). Ij (0.3 g.) and 1 g. Ba(NO3)2.H2O in 4 ml. hot H2O and the rapidly cooled solution treated with 1 ml. AcOH, kept 5 hrs. and treated with 8.06 ml. N H2SO4, the filtered solution evaporated in vacuo below 15° and the residue crystallized (4 ml. 5:2 alc.-H2O) gave 0.14 g. Ik, 8-azaxanthosine, m. 198-9° (decomposition), [α]20D -103° (c 1.02, 0.1N NaOH). The spectral characteristics of the products were tabulated [pyrimidine, λmaximum in mμ (10-3 ε) in HCl (normality indicated), at pH 6.8, and in NaOH (normality indicated) recorded]: Va, 244, 286 (5.3, 11.6, 0.1N), 246, 299 (5.5, 10.3), 245, 299 (5.3, 9.8, 0.1N); Ia, 263 (12.5, 0.1N), 280 (11.7), 280 (11.2, 0.1N); Ic, 260 (12.4, 0.1N), 279 (12.0), 278 (12.4, 0.1N); Id, 255 (9.4, 0.1N), 256 (8.8), 277 (10.5, 0.1N); VI, 260, 286 (11.5, 10.0, 0.1N), 222, 291 (21.7, 7.2), 329 (7.4, 0.1N); If, 254, 284 (9.1, 6.7, 0.1N), 258, 287 (5.1, 8.8), 259, 287 (5.1, 8.8, 0.1N); Vc, 230, 285, 303 (12.3, 13.3, 12.6, 0.05N), 223, 248, 279, 308 (15.9, 13.3, 10.5, 9.8), 248, 279, 310 (14.4, 10.3, 10.1, 0.05N); Ih, 245, 280 (13.7, 14.7, 0.05N), 248, 289 (19.4, 13.5), 247, 289 (18.9, 12.9, 0.05N); Vd, 222, 238, 287 (14.0, 14.8, 9.9, 0.05N), 219, 242, 288 (15.0, 14.3, 9.8), 244, 276, 300 (15.0, 9.8, 10.8, 0.05N); Ii, 232, 273 (9.5, 18.0, 0.05N), 242, 276 (12.5, 15.1), 242, 283 (16.8, 14.8, 0.05N); Vb, 285 (6.3, 0.01N), 238, 297 (8.4, 7.1), 254, 256, 304 (5.6, 5.6, 8.8, 0.03N); Ij, 255, 269 (13.6, 10.3, 0.01N), 256, 275 (13.7, 9.5), 221, 279 (23.0, 11.6, 0.03N); Ik, 240, 256 (5.9, 9.5, 0.1N), 252, 277 (9.7, 8.8), 251, 280 (7.1, 9.5, 0.1N); VII, 265 (15.1, 0.05N), 262 (14.8), 225, 271 (19.2, 14.8, 0.05N).

L9 ANSWER 19 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1950:18209 CAPLUS
DN 44:18209
OREF 44:3611a-b
TI A test of **triazolopyrimidines** on mouse sarcoma 180
AU Stock, C. Chester; Cavalieri, Liebe F.; Hitchings, George H.; Buckley, Sonja M.
CS Sloan-Kettering Inst., New York, NY
SO Proceedings of the Society for Experimental Biology and Medicine (1949), 72, 565-7
CODEN: PSEBAA; ISSN: 0037-9727
DT Journal
LA Unavailable
AB 5,7-Diamino-, 5-hydroxy-**7-amino**-, 5,7-dihydroxy-, **7-amino**-, and 5-**amino**-7-hydroxy-1-v-triazolo[d]-pyrimidine at tolerated doses were without inhibitory effect on sarcoma 180.

L9 ANSWER 20 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1949:6487 CAPLUS
DN 43:6487
OREF 43:1424g-i,1425a-c
TI Ultraviolet absorption spectra of purines, pyrimidines, and **triazolopyrimidines**
AU Cavalieri, Liebe F.; Bendich, Aaron; Tinker, John F.; Brown, George Bosworth
SO Journal of the American Chemical Society (1948), 70, 3875-80
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA Unavailable
GI For diagram(s), see printed CA Issue.
AB The purpose was to correlate the spectra of various substituted purines,

pyrimidines, and **triazolopyrimidines** and ascertain which functional groups are the chromophores. The homogeneity of the compds. was determined by the countercurrent distribution procedure. 2,4,5,6-Tetraaminopyrimidine sulfate (I) (9 g.) in 1500 cc. H2O at 15°, treated with 2.8 g. NaNO2 in 5 cc. H2O and the product crystallized from 2 N H2SO4 gives 2.2 g. 5,7-diamino-1H-v-triazolo[d]pyrimidine sulfate (II). 4,5,6-Triamino-2-hydroxypyrimidine sulfate (III) (10 g.) gives 2 g. **7-amino**-5-hydroxy-1H-v-triazolo[d]pyrimidine, analyzed as the HCl salt (IV) (from 6 N HCl). The absorption spectra are given as curves; the absorption maximum are listed for various pH (given in brackets) (log ε is given in each case but not reproduced here); the distribution constant (DC) was determined in BuOH-M K phosphate at pH 6.5. Adenine 264, 261, 262 [1.99, 6.47, 8.99]; 2,6-diaminopurine sulfate 282, 241, [1.97], 280, 247, 280 [6.49], 248, 280 [9.02]; isoguanine sulfate 282 [1.97], 238, 286 [6.48], 282 [8.96]; guanine sulfate 247 [1.93], 246, 275 [5.99], 245, 275 [8.80]; xanthine 266 [2.01], 268 [6.58], 240, 277 [9.02]; hypoxanthine 250, 251, 257 [1.99, 6.44, 8.82]; **7-amino** -1-v-triazolo[d]pyrimidine 265 [2.01, 6.53, 8.83]; II 252 [1.97], 251, 282 [6.49], 250, 289 [8.19]; IV 277 [2.08], 250, 277 [6.68, 8.56]; 5-**amino**-7-hydroxy isomer of IV 247 [1.98], 247, 274 [6.59, 8.43]; 5,7-dihydroxy-1-v-triazolo[d]pyrimidine 265 [1.97, 6.54, -8.45], 234, 285 [0.1 N NaOH]; 4,5,6-triaminopyrimidine 287, 279 [1.97, 6.50]; I 273 [2.20], 250, 283 [6.29]; III 280 [1.97, 6.46]; 2,4,5-triamino-6-hydroxypyrimidine sulfate 264 [1.95], 245, 275 [6.29]; 4,5-diamino-2,6-dihydroxypyrimidine sulfate 260, 273 [2.03, 6.28]; 4,5-diamino-6-hydroxypyrimidine-HCl 257, 279 [2.26, 6.30]. From the variation of the spectra with certain substituents and the similarities of the spectra of the above compds. it is apparent that the ultraviolet absorption spectra of purines are due principally to the pyrimidine moiety and that the major chromophore in the pyrimidine ring is the -C:CC:N- system.

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     (FILE 'HOME' ENTERED AT 17:11:36 ON 22 APR 2004)

     FILE 'REGISTRY' ENTERED AT 17:11:57 ON 22 APR 2004
L1             STRUCTURE UPLOADED
L2           1 S L1 SSS FULL

     FILE 'MARPAT' ENTERED AT 17:12:27 ON 22 APR 2004
L3           4 S L1 SSS FULL

     FILE 'CAOLD' ENTERED AT 17:12:39 ON 22 APR 2004

     FILE 'CAOLD' ENTERED AT 17:12:56 ON 22 APR 2004
               S L1

     FILE 'REGISTRY' ENTERED AT 17:13:02 ON 22 APR 2004
L4           1 S L1 SSS FULL

     FILE 'CAOLD' ENTERED AT 17:13:02 ON 22 APR 2004
L5           0 S L4 SSS FULL

     FILE 'CAPLUS' ENTERED AT 17:13:07 ON 22 APR 2004
L6           1 S L2
L7           4 S L3
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L8          160 S AMINO AND TRIAZOLOPYRIMIDINES
L9           20 S L8 AND  7-AMINO
L10           0 S L8 AND 4-HALOGENS
L11           0 S L8 AND 5-HALOGENS
L12           3 S L8 AND 6-PHENYL
L13           0 S L8 AND 6-ARYL

=> d l12 fbib hitstr abs total

L12  ANSWER 1 OF 3  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   1962:403998  CAPLUS
DN   57:3998
OREF 57:812i,813a-i,814a-d
TI   Contribution to the study of s-triazolopyridazines and s-
     triazolopyrimidines
AU   Libermann, David; Jacquier, Robert
CS   Lab. Carbo-Synthese, Issy-Les-Moulineaux
SO   Bulletin de la Societe Chimique de France (1962) 355-61
     CODEN: BSCFAS; ISSN: 0037-8968
DT   Journal
LA   Unavailable
OS   CASREACT 57:3998
GI   For diagram(s), see printed CA Issue.
AB   Cyclizing 2 g. 3-hydrazino-6methylpyridazine (I) with 20 cc. HCO2H (II) by
     refluxing 6 hrs. yielded 1.3 g. 6-methyl-s-triazolo[4,3-b]pyridazine
     (III), also made by condensing 4-amino-1,2,4-triazole (IV) and
     Et acetoacetate to 6-methyl-8-hydroxy-s-triazolo[4,3-b]-pyridazine (V),
     converting V to 6-methyl-8-chloro-s-triazolo[4,3-b]pyridazine (VI) with
     POCl3, and reducing VI with H (Buelow and Haas, CA 4, 2819).  III was also
     prepared from 4,4-dimethoxy-2-butanone and IV (Allen, et el., CA 54,
     19693i).  As the structure of V is known from its ultraviolet spectrum,
     this established the structure of III in accord with the interpretation of
     Buelow (CA 3, 2564) for the reaction of β-diketones of β-ketonic
     esters and IV.  VI (5 g.) and 5 cc. 98% hydrazine hydrate (VII) in 75 cc.
     alc. refluxed 1 hr. and cooled yielded 1.2 g. 6-methyl-8-hydrazino-s-
     triazolo[4,3-b]pyridazine (VIII), m. 223-5° (decomposition), after
     decolorizing and H2O repptn.  VIII (0.8 g.) and 6 cc. II was refluxed 5
     hrs., vacuum concentrated, and recrystd. twice with H2O to obtain 0.25 g.
     6-methyl-8-(formylhydrazino)-s-triazolo[4,3-b]pyridazine, m.
     267-70° (decomposition). V (14.5 g.) and 13 g. P2S5 in 450 cc. anhydrous
     pyridine was refluxed 1 hr., concentrated on a H2O bath, dissolved in a min. of
     H2O, and left 12 hrs. in a refrigerator.  The precipitate was dissolved in 60
cc.
     2N NaOH, filtered, acidified with concentrated HCl, precipitated in the
refrigerator,
     and recrystd. in 50% alc. to obtain 5.1 g. 6-methyl-8-mercapto-s-
     triazolo[4,3-b]pyridazine, m. 228-30°.  Et γ-
     phenylacetoacetate (IX) (13 g.) and 5 g.  IV in 25 cc. tetrahydro-furfurol
     (X) was heated 6 hrs. at 200°.  The vacuum concentrated residue was extracted
     several times with 7% NaHCO3 solution  The filtered extract acidified with
dilute
     HCl yielded 3 g. 6-benzyl8-hydroxy-s-triazolo[4,3-b]pyridazine, m.
     211°.  Et benzoylacetate (26 g.) and 7 g.  IV was heated at
     150° 5 hrs. 6-Phenyl-8-hydroxy-s-triazolo[4,3-
     b]pyridazine (6.5 g., m. 283°, recrystd. from 85% AcOH) solidified
     when triturated with 7 cc. H2O. s-Triazolopyrimidines.  The
     π-electrons of 3- amino-1,2,4-triazole (XI), unlike those of
     IV, were delocalized; thus, nucleophilic attack of β-oxo esters led
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to 2 isomers, XI and XII, also previously reported as the products of the reaction of 2-hydrazino-4-hydroxy-6-methylpyrimidine and II according to reaction conditions. But the 4 isomers shown (XI-XV) were theoretically possible for both reactions. XIV, hut not XV, had been isolated in the reaction of the pyrimidine and Et formate. An envisaged similar transposition of the s-triazolopyridazines, which would lead to s-triazolo[2,3-b]pyridazines, was not observed. 2-Hydrazino-4-hydroxy-6-benzylpyrimidine (XVI) (40 g.) and 250 g. II was refluxed 8 hrs., vacuum concentrated, and crystallized from H2O to obtain 25 g. product, m. 236°, which was extracted with boiling AcOBu; after each extraction, crystals were recovered, and the filtrate was used again. The combined ppts. (16.7 g.) were extracted with 2 l. boiling H2O and filtered. Two recrystns. of the precipitate from the filtrate in 350 cc. H2O yielded 2 g. 5-hydroxy-7-benzyl-s-triazolo[4,3-a]pyrimidine (XVII), m. 207-8°, λalc. 299 mμ, log ε 4.02. After 14 extns. of the AcOBu-insol. fraction with boiling BuOH, 14.3 g. 7-hydroxy-5-benzyl-s-triazolo[2,3-a]pyrimidine (XVIII), m. 236° λalc. 277 mμ, log ε 3.98, and λ 212 mμ, log ε 4.52, was collected. XI (8.4 g.), 20.6 g. IX, 40 g. X, and a few drops pyridine was heated 1 hr. at 170-80°. After vacuum concentration, the residue was extracted with NaHCO3 solution AcOH precipitated 11 g. XVIII. XV (21 g.) and 37 g. II was heated 3 hrs. at 50-60°. Excess II was evaporated below 70°. XVII was recovered similarly to XVIII above. POCl3 (55 cc.) and 5 g. XVIII was heated on a boiling H2O bath. The vacuum concentrated residue was added to crushed ice and triturated with solid Na2CO3 until the solution was alkaline The product slowly hardened. Recrystn. from 40 cc. AcOEt after filtration and the addition of 30 cc. petr. ether yielded 2 g. 7-chloro-5-benzyl-s-triazolo[2,3-a]pyrimidine (XIX), m. 103°. XIX (3.5 g.) and 2.1 g. VII in 40 cc. alc. was refluxed 3 hrs. The crystals formed upon cooling were washed with dilute Na2CO3 solution and H2O and recrystd. in 10:1 CH2Cl2-alc. to obtain 2 g. 7-hydrazino-5-benzyl-s-triazolo[2,3-a]pyrimidine (XX), m. 212°. 7-Mercapto-5-benzyl-s-triazolo[2,3-a]pyrimidine (XXI) (3.4 g.) and 3.5 g. VII was refluxed 3 hrs. in 200 cc. alc. The chilled solution was filtered and vacuum concentrated to obtain 2 g. XX.2H2O, m. 161-2°. XVIII (4.28 g.) and 5.5 g. P2S5 was refluxed 12 hrs. and poured hot into 400 cc. boiling H2O. After 2 hrs., 500 cc. ice H2O was added, the solution left overnight in a refrigerator, filtered, vacuum concentrated, and cooled to obtain 3.4 g. XXI m. 243-4° (alc.) (decomposition). 2-Hydrazino-4-hydroxy-6phenylpyrimidine (XXII) (40 g.) and 250 g. II was refluxed 6 hrs., then vacuum concentrated Boiling absolute alc. extracted 12 g. 5-hydroxy-7-phenyl-s-triazolo[4,3-a]pyrimidine (XXIII), m. 240° (iso-BuOH). The residue was 16 g. 7-hydroxy-5-phenyl-s-triazolo[2,3-a]pyrimidine (XXIV), m. 290° (iso-BuOH). XI (5 g.) and 12 g. Et benzoylacetate in 255 cc. AcOH was refluxed 2 hrs. and vacuum concentrated The water-washed residue was dissolved in NaHCO3 solution AcOH precipitated 3 g. XXIV.

XXII (20 g.) was heated with 40 g. II 4 hrs. at 50-60° and concentrated below 60°. XXIII (4.1 g.) was purified as was XXIV. The insol. fraction was 2-formylhydrazino-4-hydroxy-6-phenylpyrimidine. Refluxing 10 g. XXII in 50 g. formamide yielded 9 g. XXIV (50% HCO2H) upon cooling. XXIV (5 g.) was refluxed with 50 cc. POCl3 30 min., then vacuum concentrated The concentrate was added to crushed ice, neutralized with Na2CO3, and extracted with CHCl3. The dried extract was evaporated to give 3.5 g. 7-chloro-5-phenyl-s-triazolo[2,3-a]pyrimidine (XXV), m. 159°

(C6H6). XXV (1.3 g.) and 0.7 g. VII was refluxed 5 hrs. in 5 cc. alc.; chilling precipitated 7-hydrazino-5-phenyl-s-triazolo [2,3-a] pyrimidine (washed with Na2CO3 solution and H2O, recrystd. from alc.), m. 244-5°.

L12 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1961:54307 CAPLUS
DN 55:54307
OREF 55:10450e-i,10451a-i,10452a-h
TI Pyrimidine derivatives. IX. Mercapto-s-**triazolopyrimidines**
AU Shirakawa, Kenzo
CS Takeda Pharm. Inds. Ltd., Osaka
SO Yakugaku Zasshi (1960), 80, 1542-50
CODEN: YKKZAJ; ISSN: 0031-6903
DT Journal
LA Unavailable
AB cf. CA 54, 24761h. NaOH (1.3 g.) in 40 ml. 50% EtOH treated with 4.2 g. 2-hydrazino-4-hydroxy-6-methylpyrimidine (I) and 3 ml. CS2, the mixture refluxed 4 hrs., and the product filtered off gave Na salt of 3-mercapto-5-hydroxy-7-methyl-s-triazolo[4,3-a]pyrimidine (II); the filtrate acidified with AcOH gave 1.9 g. 3-mercapto-5-methyl-7-hydroxy-s-triazolo[4,3-a]pyrimidine (III), m. 287° (decomposition); the Na salt of II and AcOH gave the free II, m. 285° (decomposition). There was no depression of m.p. by mixing the free II and III but the Rf of free II was 0.50 and that of III was 0.62. Isomerization of the free II. Solid paraffin (5 g.) at 250-5° treated with 0.7 g. free II, the mixture kept 5 min., cooled, the paraffin extracted with C6H6, the insol. residue taken up in dilute NH4OH, acidified with AcOH, and the product filtered off gave III, m. 287° (decomposition). I (14 g.) in 500 ml. hot 50% EtOH treated with 13.5 g. PhNCS, the mixture kept overnight, the product filtered off, and washed with hot EtOH gave 24.5 g. 1-(4-hydroxy-6-methyl-2-pyrimidyl)-4-phenyl-3-thiosemicarbazide (IV), m. 277° (decomposition). IV (10 g.) and 15 g. molten paraffin at 210-20° kept 5 min., cooled, the paraffin washed with C6H6, and the insol. residue in hot H2O recrystd. (HCONH2) gave 5.6 g. III, m. 287° (decomposition). The free II (1.5 g.) in 50 ml. 1% NH4OH and 6 g. Raney Ni refluxed 1.5 hrs., the solution filtered hot, the filtrate refluxed 1 hr. with 4 g. Ni catalyst, the solution concentrated, and acidified with AcOH gave 0.7 g. 5-hydroxy-7-methyl-s-triazolo[4,3-a]-pyrimidine (V), m. 251° and 278°. III (1 g.) in 25 ml. 10% H2SO4 at 50-5° treated with 2.5 g. NaNO2, the mixture kept 10 min., and NaHCO3 added until the solution remained weakly alkaline gave 0.7 g. 5-methyl-7-hydroxy-s-triazolo[4,3-a]pyrimidine (VI), m. 300° (decomposition) (H2O). III (1 g.) in 20 ml. H2O while refluxing treated dropwise with 2.1 g. 30% H2O2, the solution concentrated, and neutralized with NaHCO3 gave 0.61 g. VI. III with Raney Ni in 1% NH4OH gave VI. III (2.6 g.) in 40 ml. 4% NH4OH at 10-13° treated with 4.8 g. KMnO4 portionwise, the solution decolorized by adding EtOH, filtered, the filtrate acidified with H2SO4, and concentrated gave 3 g. VI 3-sulfonic acid derivative, m. 300° (decomposition). 2-Hydrazino-4-hydroxy-6-phenylpyrimidine (VII) (6 g.) in 60 ml. 1:1 C5H5N-H2O and 9 ml. CS2 refluxed 10 hrs., cooled, and the product recrystd. (AcOH) gave 3.4 g. 3-mercapto-5-phenyl-7-hydroxy-s-triazolo[4,3-a]pyrimidine-AcOH (VIII), m. 258-9° (decomposition); the mother liquor from VIII concentrated and the residue recrystd. (dilute AcOH) gave

3-mercapto-5-hydroxy-7-phenyl-s-triazolo[4,3-a]pyrimidine (IX), m. 257-8° (decomposition). The separation of VIII and IX was difficult but VIII showed Rf 0.60; that of IX was 0.70. IX (1 g.) in 10 ml. 8% NaOH at 0° treated dropwise with 1.5 ml. 30% H2O2, the mixture kept a while at room temperature, heated 15 min. at 40°, cooled and the solution acidified gave 0.45 g. 5-hydroxy-7-phenyl-s-triazolo[4,3-a]pyrimidine (X), m. 237-8° and 293-4°. IX in dilute NH4OH with Raney Ni did not give X but gave β- or γ-form crystals of 2- **amino** -4-hydroxy-**6**-**phenyl**-pyrimidine, m. 303° (decomposition). VII (18.5 g.) in 500 ml. hot 80% EtOH treated with 12.5 g. PhNCS and the product filtered off gave 30 g. 1-(4-hydroxy-**6**-**phenyl**-2-pyrimidyl)-4-phenyl-3-thiosemicarbazide (XI), m. 198-202°. XI (5 g.) heated 5 min. at 250°, cooled, and the product washed with C6H6 gave 3.5 g. 2-anilino-4-hydroxy-6-phenylpyrimidine (XII), needles, m. 281° (95% AcOH). 2-Nitroamino-4-hydroxy-6-phenylpyrimidine (1 g.) and 1 ml. PhNH2 heated gently to 190° and the product washed with C6H6 gave XII, m. 280-1°. IX(0.3 g.)and 3 ml. PhNH2 refluxed 5 min. and the product washed with C6H6 gave 0.08 g. XII, m. 280-1°. 2-Hydrazino-4-hydroxy-5,6-tetramethylenepyrimidine (XIII) (3.6 g.) in 100 ml. 70% EtOH at 60° treated with 2.7 g. PhNCS in 10 ml. EtOH and heated at 60-70° gave 3.8 g. 1-(4-hydroxy-5,6-tetramethylene-2-pyrimidyl)-4-phenyl-3-thiosemicarbazide (XIV), m. 287-8° (decomposition). XIII (6 g.) in 40 ml. 1:1 C5H5N-H2O and 6 ml. CS2 refluxed 4 hrs. and the product filtered gave 2.5 g. 3-mercapto-5,6-tetramethylene-7-hydroxy-s-triazolo[4,3-a]pyrimidine (XV), plates, m. 310° (decomposition) (70% HCO2H); the mother liquor from XV concentrated gave 0.12 g. C9H10ON4S, columns, m. 296° (decomposition). XIV (10.5 g.) in 15 g. paraffin heated 10 min. at 220°, the product washed with C6H6, and the residue recrystd.(HCONH2) gave 4.8 g. XV, m. 310° (decomposition). XV (1.5 g.) in 40 ml. 1.5% NH4OH and 12 g. Raney Ni refluxed 1.5 hrs. and the product recrystd.(H2O) gave 0.21 g. 5,6-tetramethylene-7-hydroxy-s-triazolo[4,3-a]pyrimidine, needles, m. 268-70° (decomposition). The reaction of 2-hydrazino-4-hydroxy-5,6-trimethylenepyrimidine and an equivalent amount of PhNCS gave 1-(4-hydroxy-5,6-trimethylene-2-pyrimidyl)-4-phenyl-3-thiosemicarbazide (XVI), m. 285° (decomposition). XVI (6 g.) and 10 g. paraffin heated 5 min. at 215-20°, the product washed with C6H6, the insol. residue taken up in 4% NH4OH, and acidified with AcOH gave 3.9 g. 3-mercapto-5,6-trimethylene-7-hydroxy-s-triazolo[4,3-a]pyrimidine (XVII), m. 285° (decomposition). XVII (1.5 g.) and Raney Ni treated as XV above gave 0.5 g. 5,6-trimethylene-7-hydroxy-s-triazolo[4,3-a]pyrimidine, m. 301° (decomposition). 2-Hydrazino-3-benzyl-6-methyl-4(3H)-pyrimidinone (0.5 g.) in 5 ml. C5H5N and 1 ml. CS2 refluxed 15 min., an equal amount of H2O added, and the mixture cooled gave 0.54 g. 3-mercapto-5-methyl-8 benzyl-s-triazolo[4,3-a]pyrimidin-7(8H)-one, m. 315° (decomposition). 2-Hydrazino-4-hydroxy-6-methylpyrimidine (21 g.) in 80 ml. 15% NaOH at 5° treated dropwise with 18 g. ClCO2Et, the mixture kept 2 hrs., AcOH added to pH 5.5, and the product recrystd.(94% EtOH) gave 22.6 g. 2-ethoxycarbonylhydrazino derivative, m. 222°; this (1 g.) fused at 240-50° gave 0.7 g. 3,7-dihydroxy-5-methyl-s-triazolo[4,3-a]pyrimidine, m. 325° (decomposition). XIII (9 g.) in 200 ml. H2O treated with concentrated HCl to pH 4, the solution at 25° treated with 5.7 g. KCNO in 100 ml. H2O, stirred 20 min., kept overnight, and the product filtered off gave 1-(4-hydroxy-5,6-tetramethylene-2-pyrimidyl)-3-semicarbazide, needles, m. 232° (decomposition) and 300-8°; this (1.3 g.) heated 10 min. at 235-40°, the product taken up in hot AcOH, filtered with C, and diluted with H2O gave 0.9 g. 3,7-dihydroxy-5,6-tetramethylene-s-triazolo-[4,3-a]pyrimidine, m. 309° (decomposition).

2-Hydrazino-4-methylpyrimidine (6.2 g.) in 50 ml. H2O and 45 ml. 10% NaOH at 0° treated with 6.5 g. ClCO2Et portionwise and kept for a while gave 2-ethoxycarbonylhydrazino-4-methyl-pyrimidine, plates, m. 140-2° (C6H6-ligroine); this did not cyclize on heating at 250°. 2-Hydrazino-4,6-dimethylpyrimidine (6.9 g.) in 100 ml. 80% EtOH containing 2 g. NaOH and 7 ml. CS2 refluxed 2 hrs., cooled, the precipitate of 3-NaS derivative filtered off, the filtrate concentrated, and the residue acidified with AcOH gave 0.4 g. 2-HS derivative, needles, m. 255° (decomposition) (EtOH); the 3-NaS derivative in H2O acidified with AcOH gave 3.5 g. 3-mercapto-5,7-dimethyl-s-triazolo[4,3-a]pyrimidine (XVIII), needles, m. 255° (decomposition). XVIII (0.05 g.) in 10 ml. H2O boiled 10 hrs. and the products chromatographed on paper gave 0.04 g. 3-mercapto-5,7-dimethyl-s-triazolo[2,3-a]pyrimidine (XIX), m. 251° (decomposition), and a substance assumed to be 3-mercapto-5-**amino**-s-triazole. XVIII (0.03 g.) in 6 ml. 1% NaOH kept at room temperature and the product chromatographed on paper indicated the formation of XIX. 2-Hydrazino-4,6-dimethylpyrimidine (13.8 g.) in 150 ml. hot 70% EtOH treated with 13.5 g. PhNCS and left standing gave 26.3 g. 1-(4,6-dimethyl-2-pyrimidyl)-4-phenyl-3-thiosemicarbazide (XX), needles, m. 186.5° (decomposition). XX (5 g.) fused 6 min. at 195-200° and the product extracted with Et2O gave 1.7 g. XIX, m. 255° (decomposition) (MeOCH2CH2OH); the mother liquor gave 0.15 g. (PhNH)2CS, m. 151-3°. XVIII (1 g.) in 1 ml. 30% NH4OH and 23 ml. H2O refluxed 30 min. with 4 g. Raney Ni and the product concentrated gave 0.1 g. 5,7-dimethyl-s-triazolo[4,3-a]pyrimidine, needles, m. 165-7° [HC(OEt)3dioxane]. XIX (0.1 g.) in 3 ml. AcOH and 0.2 ml. 30% H2O2 refluxed 10 min., the solution concentrated, and the residue in H2O and K2CO3 extracted with C6H6 gave 0.01 g. 5,7-dimethyl-s-triazolo[2,3-a]pyrimidine, m. 135-6°. 2-Hydrazinopyrimidine (2.2 g.) in 20 ml. 80% EtOH containing 0.8 g. Na and 3 ml. CS2 refluxed 2 hrs., cooled to precipitate the Na salt of 3-mercapto-s-triazolo[4,3-a]pyrimidine (XXI), the filtrate concentrated, and the residue acidified with AcOH gave 0.1 g. 2-HS analog of XXI, plates, m. 245° (decomposition); the Na salt of XXI treated with AcOH and the product recrystd. (99% EtOH) gave 0.78 g. XXI, needles, m. 242° (decomposition). XXI isomerized to 2-mercapto-s-triazolo[2,3-a] pyrimidine (XXII) by boiling in 50% C5H5N-H2O or in H2O. 2-Hydrazinopyrimidine (5 g.) in 8 ml. CS2 and 40 ml. C5H5N refluxed 3.5 hrs., the solution filtered, the filtrate concentrated, the residue washed with H2O, taken up in dilute alkali, and acidified with AcOH gave 3.2 g. 3-mercapto-5-**amino** -s-triazole (XXIII), m. 309° (decomposition). XXIII (0.2 g.) in 10 ml. H2O treated with 0.6 g. 30% H2O2, refluxed 15 min., cooled, 0.25 g. NaHCO3 and 0.45 g. picric acid added gave 5-**amino**-s-triazole picrate, m. 229-31°. XXI (0.32 g.) in 10 ml. 1% NH4OH and 3.5 g. Raney Ni refluxed 1.5 hrs., the solution concentrated, and the residue extracted with C6H6 gave s-triazolo[2,3-a]pyrimidine, needles, m. 141-3°. 1-(2-Pyrimidyl)-4-phenyl-3-thiosemicarbazide (4.9 g.), m. 184-5° (prepared from 2-hydrazinopyrimidine and PhNCS), fused 4 min. at 190°, the product treated with 1:1 EtOH-C6H6, and filtered gave 0.8 g. XXIII, m. 308° (decomposition); the mother liquor gave 1.5 g. (PhNH)2CS, m. 151-3°. 2-Hydrazino-4-methylpyrimidine (12.4 g.) in 80 ml. 50% EtOH containing 4 g. NaOH and 10 ml. CS2 refluxed 4 hrs. and cooled gave precipitate of Na salt of 3-mercapto-5-methyl-s-triazolo[4,3-a]pyrimidine

(XXIV); the filtrate acidified with AcOH gave 3.8 g. 7-Me analog (XXV) of XXIV, m. 255° (decomposition). The Na salt of XXIV treated with dilute AcOH and the product recrystd. (70% EtOH) gave 3.1 g. XXIV, m. 255° (decomposition). XXIV and XXV showed no depression of m.p. on mixing and had the same Rf. XXIV (0.3 g.) in 1 ml. H2O and 0.3 ml. C5H5N refluxed 20 min., the solution concentrated, and the residue in 3 ml. H2O acidified gave 0.27 g. 2-mercapto-7-methyl-1,2,4-triazolo[2,3-a]pyrimidine (XXVI), prisms, m. 247° (decomposition). Similarly, XXV yielded 5-Me analog (XXVII) of XXVI, m. 249° (decomposition). XXIV (0.4 g.) in 10 ml. 1% NH4OH and 3 g. Raney Ni refluxed 1.5 hrs., the solution concentrated, the residue in 5 ml. 10% NH4OH refluxed 1.5 hrs., and the product recrystd. (C6H6-ligroine) gave 0.19 g. 7-methyl-s-triazolo[2,3-a]pyrimidine (XXVII), m. 136-8°. Similarly, 6 g. XXV yielded 1.2 g. 5-Me analog of XXVII, prisms, m. 180-2°.

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TI Structure of certain polyazaindenes. IV. Compounds from β-oxo acetals and β-methoxyvinyl ketones
AU Allen, C. F. H.; Beilfuss, H. R.; Burness, D. M.; Reynolds, G. A.; Tinker, J. F.; VanAllan, J. A.
CS Kodak Research Labs., Rochester, NY
SO Journal of Organic Chemistry (1959), 24, 796-801
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DT Journal
LA Unavailable
AB Reaction of 4,4-dimethoxy-2-butanone (I) or 4-methoxy-3-buten-2-one (II) with 3-**amino**-1,2,4-triazole (III) led to 6-methyl-1,3,3a,7-tetraazaindene (IV). The mode of formation and relation to the product from AcCH2CO2Et were discussed. This reaction of β-oxo acetals with **amino**-substituted azoles appeared to be general for the synthesis of polyazaindenes. From the above synthesis of the 4 possible products only one was obtained. These reactions were carried out in refluxing solvent with a packed column and a H2O separator, until formation of the H2O-MeOH phase was essentially complete. The product crystallized from the reaction mixts. and purified by recrystn. from the designated solvent with C. Reactions run in AcOH were refluxed 4-6 hrs. III (8.4 g.) and 33 g. 1,1,3,3-tetraethoxypropane refluxed 2 hrs. in 50 ml. AcOH containing 5 drops concentrated HCl, the solvent removed, and the residue extracted with refluxing C6H6 gave 2.9 g. crude material. Chromatography on Al2O3 followed by elution with 3:1 C6H6-CHCl3 gave 1,3,3a,7-tetraazaindene (V), m. 140-2°. II (5 g.) and 4.2 g. III in 25 ml. HCONMe2 held 18 days at 25° gave 2.4 g. prisms; an addnl. 1.4 g. of product was obtained from the mother liquors after heating 2 hrs., and concentration to a small volume The total yield of II was 3.8 g. Dimethyl sulfoxide was also used in this reaction. 4-Chloro-6-methyl-1,3,3a,7-tetraazaindene (16.9 g.), 16.9 g. MgO, 6 g. 5% Pd-C, and 200 ml. H2O shaken under 37 lb./sq. in. of H for 40 min., filtered, and the filtrate evaporated gave a solid which chromatographed on Al2O3 gave 2.7 g. pure IV. 4,4-Dimethoxy-3-methyl-1,2-butanone (VI) (12 g.) and 6.3 g. I in the xylene mixture gave 5.3 g. crystals; recrystn. gave 1.2 g. of a pure dimethyltetraazaindene(VII)and concentration of the xylene mother liquor gave 2.4 g. of an isomer (VIII). 4-Chloro-5,6-dimethyl-

1,3,3a,7-tetraazaindene prepared from the corresponding OH compound treated with MgO and Pd-C with H 1.5 hrs. at 50 lb./sq. in. gave 2.3 g. VII (5,6-dimethyl-1,3,3a,7-tetraazaindene), m. 177-8°. The crude product (11.7 g.) from the reaction run in xylene was extracted with 400 ml. hot PhCl, to yield 3.8 g. of a mixture of 2-**amino**-4-phenyl-1,3,3a,7-tetraazaindene (IX), 2-**amino**-6-**phenyl**-1,3,3a,7-tetraazaindene (X), and 2-(2-benzoylethylideneamino)-4-phenyl-1,3,3a,7-tetraazaindene (XI), which when extracted with BuOH left 0.2 g. XI, yellow solid, m. 282-3°, λ 373 mμ, ε 58,800 (CHCl3). IX (0.25 g.) was also isolated from the BuOH extract, but the bulk of the material, consisting essentially of IX and X, resisted separation A 2nd crop of 1.4 g. gave nearly pure IX, m. 268.5-9.0° (xylene), λ 339 mμ, ε 15,700 (CHCl3). The crude product (12.2 g.) from the reaction run in AcOH was fractionally crystallized to give 0.6 g. XI, 1 g. IX, and 3.1 g. X, m. 236.5° λ 311 mμ, ε 10,500 (CHCl3). XI (0.1 g.) in 50 ml. 0.1N HCl refluxed 48 hrs. and the filtrate neutralized gave platelets of IX. The reaction of I in xylene required the addition of 0.15 volume HCONMe2 to solubilize III and allow the reaction to proceed, the bulk of 6-methyl-1,2,3,3a,7-pentaazaindene (XII) separated on cooling, and the remainder was obtained by evaporation of the alc. The reaction in AcOH gave a good yield of XII directly. XII was obtained from II in 72% yield after 3 days. 2-Hydrazino-4-methylpyrimidine (4 g.) in 120 ml. H2O treated with 2 g. NaNO2 in 4 ml. H2O, followed by 4 ml. AcOH, and the mixture heated 1.5 hrs. at 90° gave 2.9 g. XII. 2-Hydrazino-4-hydroxy-6-methylpyrimidine (10 g.) and 5 g. NaNO2 in 500 ml. hot H2O was acidified with AcOH to give 5.5 g. XII. A mixture of the OH compound (50 g.) and 250 ml. POCl3 refluxed 1.2 hrs., and evaporated to dryness in vacuo, the residue treated with ice H2O, and extracted with CHCl3 gave 39.3 g. 4-chloro-6-methyl-1,2,3,3a,7-pentaazaindene (XIII), m. 106.5-7.5° (C6H6). XIII reduced in poor yield to XII. The identity of the products of all 5 methods of synthesis was shown by mixed m.ps. and by comparison of infrared and ultraviolet spectra. II (2.2 g.) and 3 g. p-O2NC6H4NHNH2 in 5 ml. HCONMe2 was left 22 hrs., and filtered to give 0.7 g. dihydrazone, m. 151-87° (decomposition) (MeCN). Heating the HCONMe2 filtrate gave 0.4 g. 3-methyl-1-p-nitrophenylpyrazole (XIV), m. 165.5°. When 0.6 g. of pure bis(p-nitrophenylhydrazone) was heated at 180-200° for 5 min. and the resulting solid recrystd., 0.25 g. pure XIV and 0.22 g. of a mixture of XIV with p-O2NC6H4NHNH2 were isolated. The following 1,3,3a,7-tetraazaindenes were thus obtained (compound number, or substituents, acetal used, azole used, reaction solvent, % yield, and m.p. given): V, 1,1,-3,3-tetraethoxypropane, III, AcOH, 22 (crude), 140-2°; IV, I, III, xylene, 63, 182.5-3.0°; IV, I, III, C6H6, 57 (crude), 173-80°; IV, I, III, AcOH, 53 (crude), 179-83°; IV, I, III, none: heat only, 66 (crude), 173-8°; IV, II, III, HCONMe2, 57, 181.5-3.0°; VII and VIII, VI, III, xylene, 69, 178-8.5° and 91-9°; 2-SMe 6-Me, I, 3-**amino**-5-methylthio-1,2,4-triazole, xylene, 65, 125-6°; 2-NH2 6-Me, I, 3,5-diamino-1,2,4-triazole, xylene, 58, 210-11.5°; IX, BzCHCH(OMe)2 (XV), 3,5-diamino-1,2,4-triazole, xylene, 95, 268.5-9.0°; X, XV, 3,5-diamino-1,2,4-triazole, AcOH, 85, 236.5°. The following miscellaneous polyazaindenes were prepared (compound no or name, acetal, azole, reaction solvent, % yield, and m.p. given): XII, I, 5-aminotetrazole (XVI), xylene-HCONMe2, 50, 133.5-4.0°; XII, I, XVI, AcOH, 91 (crude), 130-2.5°; XII, II, XVI, HCONMe2, 72, 132.5-4.0°; 5-methyl-1,2-3a,4,tetraazaindene, I, 4-**amino**-1,2,4-triazole, xylene, 16, 168-9°; 2-methyl-1,4a,9-triazafluorene, I, 2-aminobenzamidazole, xylene, 59,

233.5-4.0°; 2-**amino**-5,6,7,8-tetrahydro-1,3,3a,9-tetrazabenzotetrabenz[f]indene and (isomeric structure) compound, 2-methoxymethylenecyclohexanone, 2,5-diamino-1,2,4-triazole, xylene, 52, 317.5-18.5° and 256-64°. In the reaction involving the formation of IX, X, and XI the series of transformations was most reasonable in terms of a 1,3,3a,7-tetraaza structure (rather than a 1,2,3a,7-isomer) provided XI was formed only from the dianil, both steric hindrance and statistical influence favored the rate leading to the 1,3,3a,7-isomer. The formation of a product such as XI, in which it was evident that condensation with the 2nd mole of β-oxo acetal occurred via the acetal group and not the carbonyl, gave addnl. support to the argument regarding the 1st step in the reaction of β-oxo acetals with aminosubstituted azoles.

=> log y

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